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This thesis is dedicated to my mother Elena and my husband Victor
for their continuous support and love

Abstract

In this thesis we present two generalized methods to determine similarity solutions for the coagulation equations. The first is an indirect method applied to a quasilinear first order partial differential equation associated with the coagulation equation that determines a local Lie group of point transformations that leaves the PDE invariant. The second method is a new generalized version of the direct methods that determine the symmetry group of the point transformations to integro-differential equations. We apply this second method to the coagulation equations. These methods provide us with new family of exact and asymptotic solutions to the coagulation equations.

The group symmetry methods are further used for numerical studies. In this thesis, we focus on two classes of coagulation kernels: bounded kernels and unbounded kernels. For the class of bounded kernels we present two reliable numerical methods for solving the coagulation equation: the collocation technique, and adaptive power series method at successive points. For the class of product kernels we propose a numerical method that is very accurate and relies on combining the numerical scheme with the knowledge of the total mass or the asymptotic behaviour of solutions at large sizes.

In addition, we prove the global uniqueness of solutions to the coagulation equation with source terms in a suitable Banach space for which the global existence holds.

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Chapter 1

Introduction

We divide our introduction into five sections. In the first section, we provide some general ideas about coagulation processes. The second section describes the mathematical model for the coagulation equation with particle source terms and sinks. In the third section, we provide some motivation for studying these coagulation equations. The fourth reiterates some previous results in the mathematical theory of coagulation. Finally, in the fifth section we provide an overview of this thesis.

1.1 Coagulation processes

Disperse systems (aerosols) consisting of solid or liquid particles suspended in fluid or gas, play an important role in nature and industry. The clouds, composed of a suspension of water drops in the atmosphere, are a major factor affecting climate. The atomization of liquid fuels and the pulverization of solid fuels are common industrial operations which generate disperse systems. Many chemical materials are handled in the form of emulsions during manufacture. Many industrial operations also produce aerosols either as an intentional part of the operation or as an undesirable byproduct, such as dusts formed during mechanical processing of rocks or radioactive dust in a nuclear reactor accident and smoke evolved during the combustion of fuel.

Particulate matter processes are "emerging as a new frontier" in environmental studies as aerosols negatively affect human health, reduce visibility and modify warming through scattering and absorption of solar radiation. In general, disperse systems consist of particles of many different sizes, and knowledge of the size distribution is necessary for understanding the behaviour of the system as a whole. A better understanding of the particle size distribution of disperse systems has applications in the processing of emulsions, gas cleaning, water treatment, study of air cleaning and air pollution.

Particles in a disperse system move in response to external forces such as gravitational and electrical forces, and fluctuating forces due to thermal motion of the fluid host. This relative movement of particles can bring them into contact; when they collide and stick together, the process is called coagulation. As a result of coagulation, diffusion, and fragmentation, the particle size distribution of a disperse system changes continually. Coagulation of particles has been observed in various phenomena, such as Brownian coagulation, polymerization, as well as clustering of planets, stars and galaxies. A physical phenomenon similar to coagulation takes place in physical processes such as the growth of crystals.

The aim of this thesis is to study the particle size distribution as a function of particle size (or volume) and time as the aerosol population undergoes changes due to various physical and chemical transformations. Coagulation forms new particles of volume $\lambda + \mu$ from the collision of two particles of volumes λ and μ; the collision rate is proportional to the number of available particles and to the coagulation kernel, which will be defined below.

1.2 Mathematical model

Of particular interest to us is the coagulation process of particles in a disperse system governed by the Smoluchowski coagulation equation with particle sources and sinks:

$$\begin{aligned}\frac{\partial f}{\partial t}(\lambda, t) = \frac{1}{2}\int_0^\lambda K(\lambda-\mu,\mu)\, f(\lambda-\mu,t)\, f(\mu,t)\, d\mu - f(\lambda,t)\int_0^\infty K(\lambda,\mu)\, f(\mu,t)\, d\mu \\ + S(\lambda,t) - R(t)\, f(\lambda,t), \qquad (1.1)\end{aligned}$$

subject to initial condition

$$f(\lambda, 0) = f_0(\lambda) \qquad (1.2)$$

where the size and time variables λ, t range in $[0, \infty)$, the function $K(\lambda, \mu)$ is the coagulation coefficient for particles of sizes (or volumes) λ and μ, $S(\lambda, t)$ is the rate of addition of new particles to the system and $R(t)$ is the rate of removal of particles from the system. Each of the terms will be explained in detail below.

Equation (1.1) models a system of a large number of particles that can coagulate to form larger clusters of particles, with particle sources and sinks; each particle in the system is assumed to be fully identified by its size (or volume) λ. From a physical point of view, the basic mechanisms taken into account are the processes of particle coalescence to form larger clusters, emissions and depositions (or sources and sinks). Other effects such as multiple coagulation, fragmentation, condensation, sedimentation and spatial fluctuations are not considered. Derivations of similar equations as well as further details and examples, including a 'discrete' summation version of (1.1), can be found in Drake [25] and Dubovskii [26] and references therein.

The terms in equation (1.1) mean the following: $f(\lambda, t)$ is the density function of the particle distribution. The system is assumed to be homogeneous and unbounded and the interaction occurs only between two particles at a time. Moreover, we also assume that the total number of particles is large enough to justify the use of the density function, with $f(\lambda, t)\, d\lambda$ representing the average number of particles per unit volume having mass between λ and $\lambda + d\lambda$ at time t.

The coagulation kernel $K(\lambda, \mu)$ models the rate at which particles of mass λ coalesce with those of mass μ, and is known from the physics of the process. For physical reasons, K is assumed to be a symmetric and non-negative function. In Section 4.3 of this thesis the kernel K is also allowed to be time-dependent.

The first integral on the right-hand side of (1.1) represents the rate of increase in the number of particles of mass λ as a result of the coalescence of two particles the masses of which add up to λ. The factor 1/2 has been included to prevent double counting. The second integral represents the rate of disappearance of particles of mass λ, due to their coalescence with all other particles in the system. The function $S(\lambda, t)$ is the rate of addition of new particles into the coagulating system (the source term), and $R(t)$ determines the rate of removal of particles from the system (the sink or removal term). For physical reasons, S and R are assumed to be non-negative functions, known from the physics of the process. Neither of the functions S and R is assumed to be continuous as we would like to "turn the source and removal terms on and off" at various times. In addition, throughout the thesis, R is assumed to be a locally integrable function on an interval $[0, T) \subseteq [0, \infty)$. For a complete description of the terms in (1.1) see e.g. [25, 26, 74, 104].

For a description of physical processes, it is necessary to specify the functional forms for the coagulation coefficient $K(\lambda, \mu)$, the rate of production of new particles $S(\lambda, t)$ and the rate of particle removal $R(t)$. In a realistic environment, these functions would be complicated nonlinear functions of size (or volume) and time, which would necessitate the numerical solution of equation (1.1) in nearly all cases. Another important consideration in solving the Smoluchowski coagulation equation is a realistic choice of the initial size distribution f_0. From a physical point of view, f_0 is assumed to be non-negative, and $f_0(\lambda)\,d\,\lambda$ is the total number of particles whose volume lies between λ and $\lambda + d\lambda$ per unit volume of air.

Parameters in the coagulation equation

(i) Moments of size distribution

From a physical point of view, the following quantities are important in this thesis:

$$M_k(t) = \int_0^\infty \lambda^k f(\lambda, t)\, d\lambda, \quad \text{where} \quad k = 0, 1, 2, \ldots$$

which represent the k-th moment of the size distribution f. In particular, $M_0(t)$ is the total number of particles per unit volume at time t, $M_1(t)$ is the total mass of particles per unit volume at time t.

(ii) Coagulation kernels

The coagulation kernels we use in this thesis are those proposed by Stockmayer [108] in the chemical process of branched-chain polymerization. Stockmayer assumed that no rings can form in a polymer and every unreacted binding site has an equal chance of reacting with an available site on another polymer. With these assumptions, Stockmayer pointed out a connection of the polymer size distribution with the pure coagulation equation (1.1), where the coagulation kernel is

$$K(\lambda, \mu) = \big[(p-2)\,\lambda + 2\big]\,\big[(p-2)\,\mu + 2\big], \quad \text{where} \ \ \lambda,\ \mu \geq 0,\ \ p \geq 2.$$

Polymeric molecules (k-mers) are composed of k monomeric units. Each monomeric unit carries p functional groups which are capable of interacting with each other. Hence, the coagulation kernel K above represents the number of possible links between λ-mers and μ-mers. This kernel is physically relevant in the polymerization process where frequent branching of chains is structurally permissible. One example occurs in the glycerol-phthalic anhydride reaction, where the material gels suddenly at a certain extent of reaction independent of the temperature at which the reaction is carried out (see e.g. [108]). Stockmayer also observed that a coagulation equation with a multiplicative kernel $K(\lambda, \mu) = \lambda\,\mu$ can be obtained in fact from (1.1) in the limit $p \to \infty$ by scaling the time appropriately (by using $(p-2)^2\,t$ as a new time variable).

The coagulation kernels of interest in our thesis are given by

$$K(\lambda, \mu) = \theta(\lambda)\, \theta(\mu), \quad \text{where} \quad \theta(\lambda) = \alpha + \beta\, \lambda, \tag{1.3}$$

with α, $\beta \geq 0$ arbitrary constants. These kernels are particularly important for analyzing the "gelation" phenomenon that occurs in the case when the parameter $\beta > 0$. Examples of some commonly used coagulation kernels used in the literature and their applications can be found in [21, 22, 25, 26, 63].

(iii) Particle source terms and sinks

Source terms and sinks are potentially useful in industrial applications where one might want to exercise some control over the coagulation processes. For instance, it may be desirable to increase or restrict the limiting number of particles of a particular size. One might attempt to achieve this by the introduction of particles of some prescribed size to enable the coagulation process to arrive at some desired limiting state.

1.3 Motivation

The Smoluchowski's coagulation equation models various kinds of phenomena such as: in chemistry (polymerization), in physics (aggregation of colloidal particles, dispersion of airborne particles), in astrophysics (formation of stars and planets), in engineering (behaviour of fuel mixtures in engines), in genetics, in graph theory, etc.

The contribution of this thesis is the study of industrial processes in which particles are being added to and removed from the system while the processes occur. One example of application of such processes is the manufacturing of aluminium alloys. Here, molten metal is kept in a holding furnace for several hours while particles of titanium diboride are added for further solidification and casting. During this process these foreign particles can agglomerate and be lost from the melt by attachment to the furnace walls, thus jeopardizing the desired properties of the alloy, and increasing manufacturing costs (see, e.g. Wattis et al. [114]). Although there have been significant studies regarding the size distribution in molten aluminum, still not much is known about the kinetics of the coagulation in this system. Another application is in the study of water treatment, controlling particle mass loss is what allows the removal of tiny particles (called colloids, measured as total suspended solids) in raw water. These are just a few examples of industrial processes where one may wish to increase or modify the number of particles of a particular size. The only way to achieve this would be by the introduction or removal of particles of some prescribed size to enable the coagulation process to arrive at some desired limiting state [97].

The main purpose of this thesis is to study the dynamic behaviour of aerosol size distributions under the influence of the particle source terms and sinks.

1.4 Previous work

There is considerable literature on the mathematical theory of coagulation, both deterministic and stochastic, discrete and continuous, beginning with the pioneering work of Smoluchowski in 1917 on modeling binary coalescence of particles. Smoluchowski was the first to derive a mathematical model, assuming that the fluctuations in density were small in order that collisions occur at random. For a very comprehensive survey of work up to 1970, including applications, different derivations of the equation from physical assumptions, and discrete versions of the equation, see Drake [25]. The pioneering works of Melzak [74] (on cloud formation) include some of the earliest applications of the theory, and more applications can be found in F. da Costa [21], Drake [25], Dubovskii [26], Friedlander [45], Krivitsky [58], Lee [68], Leyvraz [63], Peterson et al [85], Zhang et al. [113], Wattis et al. [114]. The presence of external particle sources, and the removal of particles from the system, however, has not received a great deal of mathematical attention, the work of Calin et al [15, 16, 17], Dubovskii [26], Escobedo et al. [36], Lushnikov [70], Sandu et al. [90, 91], Simons [98], Shirvani et al. [97] being just a few notable recent exceptions. In [97, 98, 102], the discrete version with constant kernel and source terms is investigated. Also, solutions to the coagulation equation with a multiplicative kernel prior to the gelation have been provided in [101]. We divide this section into a few subsections in order to illustrate a few theoretical and numerical aspects that have been investigated in the literature of coagulation equations (with possible fragmentation).

1.4.1. Existence (local and global) of solutions

In papers dealing with the pure coagulation equation (without the effect of sources and sinks), the main theoretical questions are related to the study of existence and uniqueness of solutions in suitable defined Banach spaces. Almost all prior work on

Smoluchowski's equation has been established either for the case of pure coagulation or coagulation with fragmentation. Existence of solutions to the coagulation equations with possible fragmentation (the initial distribution f_0 and therefore the function f possibly enjoying additional regularity properties) have been the subject of study of several papers since the pioneering works of Aizenman and Bak [3], McLeod [73], McLaughlin et al. [72], Melzak [74], Spouge [101, 102], White [116]. Recent contributions to the existence of solutions have been brought by Calin [15], Escobedo et al. [35, 36, 38, 39], Laurençot [61], Fournier and Laurençot [42].

For bounded kernels $K(\lambda, \mu)$, global existence of solutions to the pure coagulation-fragmentation equations is investigated in [3, 8, 15, 72, 74, 95, 97]. In [16], we have extended the global existence to the case when particle sources and sinks are added into the coagulating system and for bounded, time-dependent kernels $K(\lambda, \mu, t)$. The global existence for unbounded kernels has been studied in [8, 26, 28, 39, 47, 49, 102, 103, 104, 116]. However, some authors (see e.g. [26, 47, 104]) assumed certain growth conditions on the coagulation kernel $K(\lambda, \mu)$, such as:

$$K(\lambda, \mu) \leq M\,(1 + \lambda + \mu), \ \forall (\lambda, \mu) \in \mathbb{R}_+^2, \text{ and some } M > 0. \tag{1.4}$$

For coagulation equations with fragmentation, Stewart [104] proved a general existence theorem under certain hypotheses on the growth of the coagulation and fragmentation kernels. Solutions are shown to exist in the positive cone of the Banach space defined by
$X^+ = \{f \in X : f \geq 0 \text{ a.e.}\}$, where

$$X = \{f \in L^1(0, \infty) : \int_0^\infty (1 + x)\,|f(x)|\,dx < \infty\}$$

provided that the initial distribution f_0 belongs also to X^+. Later, Laurençot [61] proved the existence of solutions to the coagulation equations with a weak fragmentation for product-type coagulation kernels in the same Banach space X^+ considered by Stewart [104]. However, a stronger notion of solution has been defined, compared to the weaker notion introduced in [104]. In [15], we have extended the global existence results for a coagulating system with particle sources and sinks.

1.4.2. Uniqueness of solutions

Global uniqueness of solutions to the pure coagulation-fragmentation has been investigated for bounded kernels in [3, 8, 15, 72, 74, 95, 97], and for unbounded kernels in

[8, 26, 28, 39, 47, 49, 73, 105]. In [16], we have extended the global uniqueness for bounded, time-dependent kernels $K(\lambda, \mu, t)$ in a coagulating system where particle sources and sinks may be included.

Norris [79] proved the local existence and uniqueness of solutions to the stochastic Smoluchowski equation for kernels $K(\lambda, \mu) \leq \varphi(\lambda)\,\varphi(\mu)$, for some continuous, sublinear functions $\varphi : (0, \infty) \to (0, \infty)$ provided that the initial distribution satisfies $\int_{(0,\infty)} \mu_0(d\lambda)\,\varphi(\lambda)^2 < \infty$.

In a recent article, Fournier and Laurençot [42] prove the uniqueness of measure-valued solutions to Smoluchowski's equations for a class of homogeneous kernels satisfying $K(u\,\lambda, u\,\mu) = u^\gamma\,K(\lambda, \mu)$, for some parameter $\gamma \in (-\infty, 2] \setminus \{0\}$ provided that the moment of order γ of the initial condition and solution are finite. The uniqueness of solutions in [42] holds in the class of measures having a finite moment of order the degree γ of homogeneity of the coagulation kernel K.

Ernst et al. [34] investigated the product kernels and proved the uniqueness of solutions by constructing explicit solutions to the pure coagulation equation by means of the Laplace transform (see also Dubovskii [26], Theorem 4.2). Using the same method, Shirvani and van Roessel [96] presented some results on the pure coagulation equation for coagulation kernels $K(\lambda, \mu)$, for $\alpha, \beta \geq 0$ defined in (1.3).

1.4.3. Conservation of mass. Gelation phenomenon

Another interesting topic has been the existence of mass-conserving solutions to the pure coagulation equation and the occurrence of gelation. A physically relevant and mathematically challenging question is to see whether the total mass of solutions to (1.1) remains constant in time, that is $M_1(t) = M_1(0)$, for all $t \geq 0$. Either formal arguments or explicit solutions have been provided to show that the conservation of mass holds true for all time $t \in \mathbb{R}_+$ in the following cases:

(i) If $K(\lambda, \mu) \leq M$, for some constant $M > 0$ and for all $(\lambda, \mu) \in \mathbb{R}_+^2$ (see [8, 72]).

(ii) If $K(\lambda, \mu) \leq C\,(\lambda + \mu + 1)$, for some constant $C > 0$ and for all $(\lambda, \mu) \in \mathbb{R}_+^2$ (see [104, 105]).

(iii) If $K(\lambda, \mu) = (\lambda\,\mu)^a$, when $a \in [0, 1/2]$ and for all $(\lambda, \mu) \in \mathbb{R}_+^2$, (see, e.g. [8, 21, 39]).

One interesting property of some coagulation equations that occurs in cases where kernels $K(\lambda, \mu)$ increase sufficiently rapidly with their sizes λ, μ is that runaway growth takes place in the system producing particles with infinite size in finite time which are removed from the system. As a result the total mass starts to decrease. In the literature this phenomenon is known as gelation, and it is interpreted physically as corresponding to the occurrence of a dynamic phase transition in the system or by the appearance of an infinite "gel" or "superparticle".

In the chemical process of polymerization, gelation can be interpreted as being the transition from polymers dissolved in solution to a gel. Roughly, one can think of a gel as a macroscopic network of polymer in solution that behaves as a solid. Theoretical investigation of the gelation phenomenon goes back to the early work of Flory [44] in 1941 and Stockmayer [108] in 1943 on condensation polymerization. Theoretical and experimental studies conducted by Flory [44] yield strong evidence that gel formation in three-dimensional polymerizations is caused by the appearance of macroscopic branched-chain molecules. More specifically, Flory analyzed the size distribution of polymers and determined theoretically the critical conditions for the formation of "infinitely large three dimensional molecules" (gel).

In the literature of coagulation, the onset of gelation has been defined by the blow up of the second moment $M_2(t)$ of the distribution (see e.g. [34, 70, 97]). There have been many reviews on models of coagulation and gelation, see e.g. Leyvraz [63]. The effect of removal terms on the gel-time was studied by Singh et al. [100], and similarly source terms were considered by Davies et al. [22].

Mathematical proofs regarding the occurrence of gelation including initial conditions for which gelation occurs, properties of the gelling solutions and classes of coagulation rates and fragmentation have been supplied recently in [21, 38, 39, 61]. Rates of decay for the zeroth and first moments of the solutions to Smoluchowski's equation are proved in [15, 36, 38, 61]. Ernst et al [34] provide asymptotic large $t \to \infty$ behaviour for the total mass $M_1(t)$. These estimates have been further applied to obtain upper and lower bounds for the gelation time, see e.g. [15, 19, 34, 38, 61, 100, 114]. Explicit gel-times and pre- and post-gelation formulas for the total mass have been provided recently in [34, 70, 89, 96]. In [89, 96], the authors provide an explicit formula for the total mass for all time $t \geq 0$ for a bilinear kernel of the form (1.3).

Ernst et al [34] prove that for the multiplicative kernel $K(\lambda, \mu) = \lambda\, \mu$, the gel-time corresponds to the first instance at which the second moment of solution defined by $M_2(t) = \int_0^\infty \lambda^2 f(\lambda, t)\, d\lambda$ diverges. This result was also shown to be true recently in [15, 97] in the absence and presence of sources for α, $\beta \geq 0$.

1.4.4. Explicit solutions

Analytical solutions to the pure coagulation equation and explicit formulas for the moments of solutions are also important in understanding the behaviour of the size distribution. However, these types of solutions have only been found for a few forms of $K(\lambda, \mu)$, including $K(\lambda, \mu) = 1$, $\lambda + \mu$, and $\lambda \mu$. Scott [94] and Ernst et al. [34] investigate the multiplicative kernel and construct explicit solutions to the pure coagulation equation by means of Laplace transforms. These solutions are also unique, see e.g. Dubovskii [26], Theorem 4.2. Also, using the saddle point method, Ernst et al [34] provide some asymptotic large size behaviour of the solution. They prove that the solution to (1.1) decays exponentially for all time $t \leq T_{gel}$, however beyond this time the solution decays algebraically.

Using the same method of Laplace transforms, and method of characteristics, Shirvani and van Roessel [96] determine necessary and sufficient conditions under which the solution to the pure coagulation equation is mass conserving. The authors consider the general coagulation kernel $K(\lambda, \mu)$ defined in (1.3). In a recent article, Lushnikov [70] provided some exact solutions to (1.1) for a product kernel $K(\lambda, \mu) = \lambda \mu$ and a constant source term under the assumption that there exist no particles at $t = 0$ (i.e. the initial size distribution $f_0(\lambda) = 0$).

Spouge [101] provided some practical solutions to the pure coagulation equation in the form of recursion and infinite series for kernels of the form $K(\lambda, \mu) = A + B(\lambda + \mu) + C \lambda \mu$ for times $t < T_{gel}$. In [15] using the method of Laplace transforms, we derived some formal series solutions to the coagulation equation with a constant kernel. Our examples include both time-dependent and time-independent examples of source terms.

Analytical solutions and their behaviour have also been provided to the discrete version of the coagulation equation in [52, 98, 110]. Dubovskii [26] obtained some properties of the equilibrium solution to the coagulation equation with a constant kernel and a time-independent source term. In addition, the author also proved the convergence of the time-dependent solution to the stationary solution.

Based on a result given by Simons [98] for the discrete equation and time-dependent source terms, in [15] we proved that the long-term behaviour of the distribution tends to be independent of the initial value and entirely determined by the source term. Questions regarding the convergence still have to be answered. For practical applications, either an analytical proof of convergence, or a numerical method of computing the inverse Laplace transform has to be used.

1.4.5. Numerical methods

In situations of practical interest, the functional forms of K, S and R are such that the time evolution of the size spectrum can only be obtained through the numerical solution of the coagulation equation. During the last century, several numerical methods have been developed for solving the coagulation equation (1.1). In the open literature, two families of methods have been developed for dealing with the coagulation equations: deterministic and stochastic. Some deterministic methods include: method of moments, finite element methods, weighted residual methods, orthogonal collocation method over finite elements, discretized population balances, finite difference methods, mesh techniques, finite volume methods, power series solutions, etc. A survey of popular numerical methods is given in [25, 59, 88, 113]. In Section 5.1 we have detailed some of the numerical methods described above. Among the variety of stochastic methods, the mass flow algorithm developed originally by Babovsky in [6] and then developed further by Eibeck and Wagner [31] is one of the most accurate methods as it provides convergence of the solution after the gelation time, which is difficult to capture with deterministic methods.

1.4.6. Asymptotics and self-similarity

Numerical simulations have confirmed that the size distribution function f should approach a mass-conserving self-similar function f_S for large times t. More precisely, the so-called dynamical scaling hypothesis predicts that for homogeneous coagulation kernels K such that $K(u\,\lambda, u\,\mu) = u^a\,K(\lambda,\mu)$, for some exponent a, where u, λ, $\mu > 0$, we have

$$f(\lambda,t) \sim f_S(\lambda,t) = s(t)^{-\tau}\,\psi\big(\lambda/s(t)\big) \tag{1.5}$$

where $s(t)$ represents the mean particle size at time $t > 0$, ψ is a non-negative function and f_S is a self-similar solution to (1.1). The assertion (1.5) goes back to Friedlander [45] and van Dongen and Ernst [24] for pure coagulation equations, however no rigorous proofs were given with respect to the existence of ψ or convergence (1.5). The first approach to self-similarity (or dynamical scaling) has been established rigorously for pure coagulation equation for the kernel $K = 2$ by Kreer and Penrose

[57]. The authors recognize the importance of the use of the Laplace transform. Menon and Pego [75, 76] extend the approach to self-similarity to a larger class of solvable, homogeneous kernels including $K = \lambda + \mu, \lambda\,\mu$. In [57], the importance of the use of the Laplace transform was recognized. In 2005, Fournier and Laurençot [43] proved the existence of at least one scaling profile ψ for three classes of homogeneous kernels with degree of homogeneity $\gamma < 1$. The existence of self-similar solutions for some other classes of kernels appears in [37]. Self-similar solutions are interesting particular solutions as they may describe the behaviour of the general solutions of the coagulation equations [24, 35, 36]. For a summary of self-similar solutions see Section 4.1 in this thesis.

1.4.7. Lie-group theoretic methods

In the recent theory of fragmentation equations a new direction has emerged: a general method for the determination of Lie groups of point transformations. Zawistowski [112] was the first to extend the method of Ovsiannikov [81] for differential equations to integro-differential equations. A generalized version of the direct methods has been given recently by Akhiev and Özer [4] to determine symmetry groups for the collisionless Boltzmann equation. The authors also propose a new approach to solve the nonlocal determining equations. For the fragmentation equation with continuous mass-loss, Elhanbaly [32] obtained the symmetry groups and a complete classification of all possible non-trivial similarity solutions.

The main purpose in this thesis is to propose a generalized method in order to derive a Lie symmetry group of point transformations for the coagulation equation in the absence/presence of particle source terms. Our aim is to obtain a new family of similarity solutions to the coagulation equation for a (non)-homogeneous kernel.

1.5 Thesis Overview

In this thesis we conduct a theoretical analysis in the field of the coagulation equations with particle sources and sinks. The thesis is divided into seven chapters. Our main goal in this section is to provide a summary of each of the subsequent chapters in the thesis.

In Section 2.1, using the technique of re-scaling the time variable t, the general Smoluchowski coagulation equation (1.1) is simplified to a coagulation equation with source terms only. In Section 2.2, we prove the global uniqueness of solutions to the coagulation equation with source terms (2.8) subject to (2.9) in the same Banach space used in Calin [15] for which we proved the global existence result.

In Chapter 3 we summarize a few facts from Lie theory, providing a brief summary of the theory of one-parameter Lie groups of point transformations and some generalized symmetries for general partial differential equations with one dependent variable and two independent variables.

In Section 4.1 we summarize a few self-similar solutions that have been obtained for the pure coagulation equation. Following the general description in Chapter 3, this thesis continues with some new approaches in the theory of coagulation equations. In Section 4.2, we provide the group analysis for a new form of a quasilinear first order partial differential equation associated to the coagulation equation in the presence of particle source terms. This analysis provides us with similarity (group-invariant) solutions and asymptotic behaviour of solutions to the coagulation equations with particle source terms as $\lambda \to \infty$ for a few special classes of initial conditions and a bilinear separable coagulation kernel in the pre- and post-gelation stages. For some special values of the parameters, we also obtain the expression of the total mass of the solution for all $t \geq 0$ and the gelation time. In Section 4.3, we apply a new generalized version of the direct methods that determine the symmetry group of point transformations for integro-differential equations to the coagulation equation in the presence of source terms. These methods yield new family of similarity solutions to the coagulation equations which can be further used for numerical studies.

Section 5.1 summarizes a family of deterministic numerical methods existing in the literature for solving the coagulation equation. We also point out some of the advantages and disadvantages that each method brings, and the classes of kernels that each of these methods solve. In Section 5.2, we present two reliable numerical methods for solving the coagulation equation that are most suitable (reliable) for a class of bounded kernels with particle source terms: the collocation technique, and adaptive power series method at successive points. In Section 5.3, we present a numerical method for a class of unbounded kernels.

In Chapter 6 we propose new future directions and steps that we need to complete in order to generalize the methods proposed in this thesis. Chapter 7 includes the proofs of some of the theorems in Section 4.2.

Chapter 2

Existence and Uniqueness of Solutions

In this chapter we are interested in studying the global existence and uniqueness of solutions to the Smoluchowski coagulation equation with source terms.

2.1 Coagulation equations with sources. Technique of rescaling

Let $f(\lambda, t)$ be the concentration (or the density function) of clusters of size λ at time t and assume that the rate K at which clusters of particles coalesce is independent of time t. Then the coagulation equation with particle source terms and sinks is given by

$$\begin{aligned}\frac{\partial f}{\partial t}(\lambda, t) = \frac{1}{2}\int_0^\lambda K(\lambda-\mu, \mu) f(\lambda-\mu, t) f(\mu, t)\, d\mu \,-\, f(\lambda, t)\int_0^\infty K(\lambda, \mu) f(\mu, t)\, d\mu \\ +\, S(\lambda, t) - R(t)\, f(\lambda, t) \qquad (2.1)\end{aligned}$$

subject to the initial condition

$$f(\lambda, 0) = f_0(\lambda) \qquad (2.2)$$

where the size variable λ and the time variable t range in $[0, \infty)$.

For the purpose of this chapter, we assume the rate K is a symmetric, bilinear function given by

$$K(\lambda, \mu) = \theta(\lambda)\,\theta(\mu), \quad \text{where} \quad \theta(\lambda) = \alpha + \beta\,\lambda,\ \forall\,\lambda \geq 0 \qquad (2.3)$$

with α, β any positive real numbers. The coagulation kernel K above includes the constant and the product kernel as special cases.

The main objective of the present section is to obtain, using a technique of rescaling the time variable t, a new but simplified form of Smoluchowski coagulation equation with particle source terms only. Indeed, multiply (2.1) by $H(t) := \exp\left(\int_0^t R(s)\,ds\right)$ and let $w(\lambda, t) := f(\lambda, t)\,H(t)$. We obtain

$$H(t)\,\frac{\partial w}{\partial t}(\lambda, t) = \frac{1}{2}\int_0^\lambda K(\lambda-\mu, \mu)w(\lambda-\mu, t)w(\mu, t)\,d\mu - w(\lambda, t)\int_0^\infty K(\lambda, \mu)w(\mu, t)\,dy + H^2(t)\,S(\lambda, t) \tag{2.4}$$

subject to the initial condition

$$w(\lambda, 0) = f(\lambda, 0)H(0) = f_0(\lambda).$$

We can rescale the time variable further. For this purpose, we introduce a new parameter $\tau = F(t)$, where the function $F(t)$ is chosen such that it satisfies the initial value problem

$$F'(t) = \frac{1}{H(t)} \quad \text{with initial condition} \quad F(0) = 0.$$

Next, define $c(\lambda, \tau) := w(\lambda, t)$ and $g(\lambda, \tau) := [H(F^{-1}(\tau))]^2\,S(\lambda, F^{-1}(\tau)) \geq 0$. Hence, we obtain the following form of the coagulation equation with source terms, where we rename τ to t

$$\frac{\partial c}{\partial t}(\lambda, t) = \frac{1}{2}\int_0^\lambda K(\lambda-\mu, \mu)c(\lambda-\mu, t)c(\mu, t)\,d\mu - c(\lambda, t)\int_0^\infty K(\lambda, \mu)c(\mu, t)\,d\mu + g(\lambda, t) \tag{2.5}$$

subject to the initial condition

$$c(\lambda, 0) = c_0(\lambda) = f_0(\lambda).$$

Therefore, any coagulation equation (2.1) with particle source terms and removal terms $R(t)$, where R is an arbitrary, non-negative function of t such that $R(t)$ is locally integrable (for definition see e.g. [15]) can be simplified to a coagulation equation (2.5) with particle source terms only by rescaling the time variable t. For this reason, in the remainder of this thesis we only consider coagulation equations with particle source terms of the form (2.5).

2.2 Uniqueness of solutions

Our main purpose in this section is to prove the global uniqueness of solutions to the coagulation equation for the case when the initial data c_0, and the source term $g(\lambda, t)$ satisfy certain assumptions and the coagulation kernel is a bilinear, non-homogeneous function.

For this purpose, consider the coagulation equation with particle source terms (2.5) given in Section 2.1, where we assume the coagulation kernel $K(\lambda, \mu)$ is of the following form

$$K(\lambda,\mu) = \theta(\lambda)\,\theta(\mu), \quad \text{where } \theta(\lambda) = \alpha + \beta\,\lambda,\ \forall\,\lambda \geq 0, \tag{2.6}$$

with $\alpha,\ \beta > 0$ any strictly positive real numbers. One can easily prove that any coagulation kernel $K(\lambda, \mu)$ of the form (2.6) can be reduced to the coagulation kernel $\Psi(\lambda, \mu) = \xi(\lambda)\,\xi(\mu)$, where $\xi(\lambda) = 1 + \lambda$. Indeed, if we rescale the size and time variables and denote by

$$u(\lambda,t) := c\Big(\frac{\alpha}{\beta}\,\lambda, \frac{\alpha^3}{\beta}\,t\Big) \quad \text{and} \quad p(\lambda,t) := \frac{\beta}{\alpha^2}\,g\Big(\frac{\alpha}{\beta}\,\lambda, \frac{\alpha^3}{\beta}\,t\Big)$$

and

$$\Psi(\lambda,\mu) := \xi(\lambda)\,\xi(\mu), \quad \forall\,(\lambda,\,\mu) \in \mathbb{R}^2_+ \quad \text{where} \quad \xi(\lambda) = 1 + \lambda. \tag{2.7}$$

Then the coagulation equation with particle source terms takes the following form

$$\frac{\partial u}{\partial t}(\lambda,t) = \frac{1}{2}\int_0^\lambda \Psi(\lambda-\mu,\mu)u(\lambda-\mu,t)u(\mu,t)\,d\mu - u(\lambda,t)\int_0^\infty \Psi(\lambda,\mu)u(\mu,t)\,d\mu + p(\lambda,t) \tag{2.8}$$

subject to the initial condition

$$u(\lambda,0) = u_0(\lambda). \tag{2.9}$$

In the existing literature on the coagulation equations, the main theoretical questions are related to the study of existence and uniqueness of solutions in suitable defined Banach spaces. The proof of existence of solutions to the coagulation equations with particle source terms (2.8) in a suitable less complicated Banach space and for a non-homogeneous coagulation kernel of the form (2.7) has already been the subject of study in [15]. However, as pointed out in Section 1.4, the proof of uniqueness of solutions to (2.8) for such a coagulation kernel was left as an open problem in [15];

and to our knowledge the proof of uniqueness for such a kernel in the presence of sources and sinks has not been proved yet (from a deterministic point of view).

In a recent article, Fournier and Laurençot [42] prove the uniqueness of measure-valued solutions to Smoluchowski's equations for a class of homogeneous kernels satisfying $K(u\,\lambda, u\,\mu) = u^{\gamma}\,K(\lambda,\mu)$, for some parameter $\gamma \in (-\infty, 2] \setminus \{0\}$ provided that the moment of order γ of the initial condition and solution are finite. However, the class of kernels considered in [42] does not cover the non-homogeneous coagulation kernels (2.7) of interest in this thesis.

Our main purpose in this section is to prove the global uniqueness of solutions to the coagulation equation with source terms (2.8) subject to (2.9) in the Banach space X_ξ, and for the non-homogeneous coagulation kernel Ψ defined by (2.7). For this purpose, we consider the same Banach space X_ξ used in [15] for which we proved the global existence result, i.e.

$$X_\xi = \{f \in L^1(0,\infty) : \|f\|_\xi < \infty\} = L^1(0,\infty; \xi(\lambda)\,d\lambda) \tag{2.10}$$

endowed with the norm $\|\cdot\|_\xi$ defined by

$$\|f\|_\xi = \int_0^\infty \xi(\lambda)\,|f(\lambda)|\,d\lambda \quad \text{for} \quad f \in X_\xi \tag{2.11}$$

where $\xi(\lambda) = 1 + \lambda$. Let X_ξ^+ be the positive cone of X_ξ, i.e. $X_\xi^+ = \{f \in X_\xi : f \geq 0 \; a.e.\}$.

Let $T \in (0,\infty]$ be arbitrary. We denote by $C([0,T]; L^1(0,\infty))$ the space of continuous functions from $[0,T]$ into $L^1(0,\infty)$ endowed with the usual sup-norm (or uniform norm) $\|\varphi\|_\infty = \sup_{t\in[0,T]} |\varphi(t)|$ (see Edwards [30], p.77). As usual the strong convergence in $L^1(0,\infty)$ is be denoted by $\rightarrow$. Full details about this type of convergence can be found in [29, 30].

Assumptions for $u_0(\lambda)$ and $p(\lambda,t)$

A1. The initial distribution $u_0 \in X_\xi^+$.

A2. The source term $p(\lambda,t)$ is a non-negative function of λ, $t \geq 0$ and satisfies the following hypothesis:

$$t \mapsto \int_0^\infty \xi(\lambda)\,p(\lambda,t)\,d\lambda \in L^\infty(0,T) \tag{2.12}$$

Before stating any result let us define the notion of solution to the coagulation equation (2.8), (2.9) that will be used further:

Definition 1 *Let $T \in (0, \infty]$ be arbitrary. A solution u of the equation (2.8) is a function $u : [0, T) \to X_\xi^+$ such that for every $t \in (0, T)$, there holds*

(a) $u \in C([0, t]; L^1(0, \infty)) \cap L^\infty(0, t; X_\xi)$

(b)

$$(\lambda, t) \mapsto \xi(\lambda) u(\lambda, t) \in L^1\big((0, \infty) \times (0, t)\big) \tag{2.13}$$

(c) *For almost every $\lambda \in [0, \infty)$:*

$$\begin{aligned} u(\lambda, t) = u_0(\lambda) + \int_0^t p(\lambda, s)\, ds + \frac{1}{2} \int_0^t \int_0^\lambda \Psi(\lambda - \mu, \mu) u(\lambda - \mu, s) u(\mu, s)\, d\mu\, ds \\ - \int_0^t u(\lambda, s) \int_0^\infty \Psi(\lambda, \mu) u(\mu, s)\, d\mu\, ds \end{aligned} \tag{2.14}$$

with u_0 and p satisfying the assumptions A1 and A2, respectively. For our definition of solution we impose the same strong property (b) as suggested in [61].

Theorem 2.1 ***(Global existence and uniqueness of solutions to (2.8), (2.9))*** *Assume the coagulation kernel Ψ is as in (2.7) and the source term p satisfies A2. For every u_0 satisfying A1, there exists a unique (strong) solution $u \in X_\xi^+$ to the equation (2.8) on $[0, T]$ for every $T \in (0, \infty)$ with $u(0) = u_0$ satisfying*

$$M_1(t) \le M_1(0) + \int_0^t \int_0^\infty \lambda\, p(\lambda, s)\, d\lambda\, ds \quad \textit{for every} \quad t \in [0, T] \tag{2.15}$$

Proof. The global existence of solutions to the coagulation equation (2.8) has already been the subject of study in [15]. So, in this thesis we only prove the uniqueness of solutions. The proof of uniqueness follows by means of a contradiction argument, and is based on the use of Laplace transforms. To our knowledge, the idea for the proof of uniqueness we present below has not been proposed in the literature of coagulation, so far. To prove uniqueness of solutions we assume that there are two distinct solutions $u(\lambda, t)$ and $v(\lambda, t)$ to the initial value problem (2.8), (2.9) with the same initial data $u(\lambda, 0) = v(\lambda, 0)$.

Let us denote their difference by $D(\lambda,t) := u(\lambda,t) - v(\lambda,t)$. Then, we have

$$\begin{aligned}\frac{\partial D}{\partial t}(\lambda,t) &= \frac{1}{2}\int_0^\lambda \Psi(\lambda-\mu,\mu)D(\lambda-\mu,t)D(\mu,t)\,d\mu - v(\lambda,t)\int_0^\infty \Psi(\lambda,\mu)D(\mu,t)\,d\mu \\ &\quad - D(\lambda,t)\int_0^\infty \Psi(\lambda,\mu)D(\mu,t)\,d\mu - D(\lambda,t)\int_0^\infty \Psi(\lambda,\mu)v(\mu,t)\,d\mu \\ &\quad + \int_0^\lambda \Psi(\lambda-\mu,\mu)D(\lambda-\mu,t)v(\mu,t)\,d\mu \qquad (2.16)\end{aligned}$$

Multiply (2.16) by $\xi(\lambda)$ and let $R(\lambda,t) := D(\lambda,t)\,\xi(\lambda)$, where $\xi(\lambda) = 1+\lambda$. Therefore, we obtain

$$\begin{aligned}\frac{\partial R}{\partial t}(\lambda,t) &= \frac{\xi(\lambda)}{2}\int_0^\lambda R(\lambda-\mu,t)R(\mu,t)\,d\mu + \xi(\lambda)\int_0^\lambda R(\lambda-\mu,t)\xi(\mu)v(\mu,t)\,d\mu \\ &\quad - \xi(\lambda)R(\lambda,t)\int_0^\infty R(\mu,t)\,d\mu - \xi(\lambda)R(\lambda,t)\int_0^\infty \xi(\mu)v(\mu,t)\,d\mu \\ &\quad - \xi^2(\lambda)v(\lambda,t)\int_0^\infty R(\mu,t)\,d\mu \qquad (2.17)\end{aligned}$$

Next, we denote by

$$Y(z,t) := \mathcal{L}\{R(\lambda,t)\}(z,t) = \int_0^\infty e^{-z\lambda}R(\lambda,t)\,d\lambda, \quad \text{where} \quad z \in [0,\infty)$$

$$P(t) := \int_0^\infty \xi(\mu)v(\mu,t)\,d\mu \geq 0 \quad \text{and} \quad Q(t) := \int_0^\infty R(\mu,t)\,d\mu = Y(0,t)$$

where, as usual $\mathcal{L}\{...\}$ denotes the Laplace transform. Formally apply Laplace transforms to the equation (2.17) to obtain

$$\begin{aligned}\frac{\partial Y}{\partial t}(z,t) &= \frac{1}{2}\mathcal{L}\Big\{\xi(\lambda)(R*R)(\lambda,t)\Big\}(z,t) + \mathcal{L}\Big\{\xi(\lambda)(R*(\xi\, v))(\lambda,t)\Big\}(z,t) \\ &\quad - \big(P(t)+Q(t)\big)\,\mathcal{L}\Big\{\xi(\lambda)R(\lambda,t)\Big\}(z,t) - Q(t)\,\mathcal{L}\Big\{\xi^2(\lambda)v(\lambda,t)\Big\}(z,t) \qquad (2.18)\end{aligned}$$

We take each Laplace transform in (2.18) separately and using Laplace transform properties we obtain

$$\mathcal{L}\Big\{\xi(\lambda)\,(R*R)(\lambda,t)\Big\}(z,t) = Y^2(z,t) - 2\,Y(z,t)\frac{\partial Y}{\partial z}(z,t) \qquad (2.19)$$

$$\mathcal{L}\{\xi(\lambda)(R*(\xi\, v))(\lambda,t)\}(z,t) = G(z,t)Y(z,t) - \frac{\partial Y}{\partial z}(z,t)F(z,t) \qquad (2.20)$$

$$\mathcal{L}\{\xi(\lambda)\,R(\lambda,t)\}(z,t) = Y(z,t) - \frac{\partial Y}{\partial z}(z,t) \qquad (2.21)$$

$$\mathcal{L}\{\xi^2(\lambda)v(\lambda,t)\}(z,t) = F(z,t) - \frac{\partial F}{\partial z}(z,t) = G(z,t), \qquad (2.22)$$

where, we denote by

$$F(z,t) := \mathcal{L}\{\xi(\lambda)v(\lambda,t)\}(z,t) = \int_0^\infty e^{-z\lambda}\xi(\lambda)v(\lambda,t)\,d\lambda \quad \text{and}$$
$$G(z,t) := F(z,t) - \frac{\partial F}{\partial z}(z,t).$$

The function $G(z,t)$ is well-defined for $z > 0$ and $t \geq 0$. Furthermore, $G(0,t)$ is only well-defined for $t < \min\{T_{gel}(u), T_{gel}(v)\}$, where $T_{gel}(u)$ denotes the time when gelation occurs for the coagulation equation in u. From the definition of $F(z,t)$ it follows that $P(t) = F(0,t)$. Substituting all (2.19 - 2.22) into (2.18) we obtain

$$\begin{aligned}\frac{\partial Y}{\partial t}(z,t) = \frac{1}{2}\left\{Y^2(z,t) - 2Y(z,t)\frac{\partial Y}{\partial z}(z,t)\right\} + Y(z,t)G(z,t) - \frac{\partial Y}{\partial z}(z,t)F(z,t)\\ - (P(t)+Q(t))\left\{Y(z,t) - \frac{\partial Y}{\partial z}(z,t)\right\} - Q(t)G(z,t)\end{aligned}$$

Therefore, $Y(z,t)$ satisfies the following P.D.E.

$$\begin{aligned}\frac{\partial Y}{\partial t} + \frac{\partial Y}{\partial z}\left\{Y(z,t) + F(z,t) - Q(t) - P(t)\right\} = \frac{1}{2}Y^2(z,t)\\ + Y(z,t)\left\{G(z,t) - P(t) - Q(t)\right\} - Q(t)G(z,t) \quad (2.23)\end{aligned}$$

It is worth pointing out that the P.D.E. (2.23) is on the domain $(z,t) \in (0,\infty)\times(0,\infty)$. Also, no boundary condition is required at $z = 0$ since

$$Y(z,t) + F(z,t) - Q(t) - P(t)\Big|_{z=0} = 0.$$

Since $D(\lambda,0) = u_0(\lambda) - v_0(\lambda) = 0$ we have $R(\lambda,0) = 0$. Hence, the partial differential equation (2.23) has the initial condition $Y(z,0) = \mathcal{L}\{R(\lambda,0)\}(z,0) = 0$. The initial value problem derived above is not a standard one since the PDE (2.23) has coefficients that are not completely known functions, such as $Q(t)$ and $P(t)$ which depend on the solution.

To prove the uniqueness of solutions to the coagulation equation (2.8) we investigate the solution $Y(z,t)$ of the P.D.E. (2.23) above. Our method of proof is as follows: Using a contradiction argument, we show that the solution of the PDE (2.23) does not have a shock at any point, in other words the gradient of the solution $Y(z,t)$ does not blow up at any time t. Having proved this assertion we can then conclude by using the method of characteristics that the system of characteristic equations associated to the PDE (2.23) can always be inverted (for every time $t \geq 0$). This statement yields the conclusion that the PDE (2.23) has a unique solution with I.C. zero, that is the trivial solution $Y(z,t) = 0$, for all time $t \geq 0$. The latter will eventually lead to a contradiction with our assumption at the beginning of the proof (that (2.8) has two distinct solutions u and v).

First, we show that the solution of the PDE (2.23) does not have a shock at any point. Indeed, assume otherwise, i.e. assume there exists a time $T_b \in [0,\infty)$ at which the gradient $|Y_z(z,T_b)| = \infty$, but $|Y_z(z,t)|$ stays finite for all $t \in [0,T_b)$, where $T_b := \inf\{t > 0 \quad s.t. \quad \|Y_z(\cdot,t)\|_\infty = \infty\}$. The characteristic equations associated to the first order partial-differential equation (2.23) with the initial condition $Y(z,0) = 0$ are given by

$$\frac{dZ}{dt} = W - Q(t) + F(Z,t) - P(t) \qquad Z|_{t=0} = \gamma \tag{2.24}$$

$$\frac{dW}{dt} = \frac{1}{2}W^2 + W\left[G(Z,t) - P(t) - Q(t)\right] - Q(t)G(Z,t) \qquad W|_{t=0} = 0, \tag{2.25}$$

where we denote by $Z = Z(\gamma,t)$ and $W = W(\gamma,t)$ the solution of the characteristic system (2.24-2.25) satisfying the initial conditions $Z(\gamma,0) = \gamma$ and $W(\gamma,0) = 0$, respectively. In addition, we assume that the functions on the right hand sides above are continuously differentiable.

From the conditions $Q(t) = Y(0,t)$ and $P(t) = F(0,t)$, if we set $z = 0$ in (2.23) then we obtain an IVP for $Q(t)$ of the following form

$$\frac{dQ(t)}{dt} = -\frac{1}{2}Q^2(t) - P(t)Q(t) \qquad \text{subject to I.C. } \mathrm{Q(0) = Y(0,\,0) = 0}. \tag{2.26}$$

From the assumption above, this I.V.P. is valid only for values of $t \in [0,T_b)$ such that both gradients $\partial F/\partial z$ and $\partial Y/\partial z$ are finite. On the one hand, it has already been proved in [15, 96] that the breaking time (or shock time) for the pure coagulation equation (2.8) ($p(\lambda,t) = 0$) corresponds in fact to the time at which the gradient of the Laplace transform of the solution $\xi(\lambda)\,u(\lambda,t)$, or $U_z(z,t)$ becomes unbounded. In addition, it was proved in [15, 96] that the breaking time T_b coincide in fact with the gelation-time. Based on the assumption at the beginning of the proof, that the equation (2.8) does not have a unique solution, this means that both solutions $\xi(\lambda)\,u(\lambda,t)$ and $\xi(\lambda)\,v(\lambda,t)$ have the gradients of their Laplace transforms, that is $U_z(z,t)$ and $V_z(z,t)$ unbounded at $t = T_b$.

On the other hand, the ODE in (2.26) is a Ricatti equation and it can be solved exactly in terms of $P(t)$. One particular solution to the I.V.P. is $Q(t) = 0$, for $t \in [0,T_b)$. Using the existence and uniqueness results for ODEs one can easily prove that $Q(t) = 0$ is indeed the unique solution to the I.V.P. (2.26) for all $t \in [0,T_b)$.

Having proved that $Q(t) = 0$, for all values of $t \in [0, T_b)$, we show next that this implies that the function $Y(z,t) = 0$, for all $t \in [0, T_b)$. Indeed, since $Q(t) = 0$ then the equation (2.25) in the characteristic system becomes

$$\frac{dW}{dt} = \frac{1}{2} W^2 + W \left[G(Z,t) - P(t)\right], \qquad \text{subject to} \quad W(0) = 0.$$

This is a Ricatti equation and either solving it or using again existence and uniqueness theorems for ODEs it can be proved that this equation has a unique solution, that is the trivial solution, or $w = W(z,t) = 0$. Therefore, the solution $Y(z,t)$ of the Cauchy problem becomes $Y(z,t) = 0$, provided that $t < \min\{T_{gel}(u), T_{gel}(v)\}$, $T_{gel}(u) > 0$ and $T_{gel}(v) > 0$. Hence, the inverse Laplace transform of $Y(z,t)$ also equals zero, i.e. $R(\lambda,t) = \xi(\lambda)\,[u(\lambda,t) - v(\lambda,t)] = 0$, for all $t < \min\{T_{gel}(u), T_{gel}(v)\}$ and $\lambda \geq 0$. Consequently, we obtain that

$$u(\lambda,t) = v(\lambda,t), \ \forall t < \min\{T_{gel}(u), T_{gel}(v)\} \quad \text{and} \quad \lambda \geq 0.$$

However, the latter contradicts our assumption and thus the uniqueness of solutions to (2.8) holds for all $t \leq T_b$ and $\lambda \geq 0$. Our next step is to prove that $Y_z(z, T_b) = 0$, for $z > 0$. This follows since $\lambda\, e^{-z\lambda} \in L^1(0,\infty)$ and $R(\lambda,t) \to 0$ as $t \to T_b$ a.e. as a consequence of the continuity of the solutions u and v. The Lebesgue dominated convergence theorem then readily implies

$$\lim_{t \to T_b^-} \int_0^\infty \lambda\, e^{-z\lambda}\, R(\lambda,t)\, d\lambda = 0, \quad \text{for } z > 0.$$

Therefore, $|Y_z(z,t)| < \infty$ for any $z > 0$, provided that $T_b > 0$. Thus, there is no time t at which the gradient $Y_z(z,t)$ would become infinite. It remains only to prove that $Y_z(z,t)$ stays finite also at $z = 0$ for all $t \geq 0$. We leave the latter for future work. Then we obtain that there is no shock time for the solution of the PDE (2.23). Therefore, one can write the characteristic equations (2.24-2.25) for all $0 \leq t < \min\{T_{gel}(u), T_{gel}(v)\}$ and these equations can always be inverted for such time t. Moreover, the function $Q(t)$ is now given by the ODE (2.26).

Next, we return to the equation (2.16) above and using the information on $Q(t) = 0$ for all $t \in [0, T_b]$ we rewrite (2.16) in the following form

$$\frac{\partial D}{\partial t}(\lambda,t) = \frac{1}{2} \int_0^\lambda \Psi(\lambda - \mu, \mu)\left[u(\lambda - \mu, t) u(\mu,t) - v(\lambda - \mu, t) v(\mu, t)\right] d\mu$$

$$
\begin{aligned}
&- \int_0^\infty \Psi(\lambda,\mu)\,[u(\lambda,t)u(\mu,t) - v(\lambda,t)v(\mu,t)]\,d\mu \\
&= \frac{1}{2}\int_0^\lambda \Psi(\lambda-\mu,\mu)\Big\{[u(\lambda-\mu,t) - v(\lambda-\mu,t)]u(\mu,t) + [u(\mu,t) - v(\mu,t)]v(\lambda-\mu,t)\Big\}\,d\mu \\
&- \int_0^\infty \Psi(\lambda,\mu)[u(\lambda,t) - v(\lambda,t)]\,u(\mu,t)\,d\mu - \int_0^\infty \Psi(\lambda,\mu)[u(\mu,t) - v(\mu,t)]\,v(\lambda,t)\,d\mu
\end{aligned}
$$

Hence,

$$
\begin{aligned}
\frac{\partial D}{\partial t}(\lambda,t) &= \frac{1}{2}\int_0^\lambda \Psi(\lambda-\mu,\mu)D(\lambda-\mu,t)u(\mu,t)\,d\mu + \frac{1}{2}\int_0^\lambda \Psi(\lambda-\mu,\mu)v(\lambda-\mu,t)D(\mu,t) \\
&\quad - D(\lambda,t)\int_0^\infty \Psi(\lambda,\mu)u(\mu,t)\,d\mu - v(\lambda,t)\int_0^\infty \Psi(\lambda,\mu)D(\mu,t)\,d\mu \qquad (2.27)
\end{aligned}
$$

Since

$$
\int_0^\lambda \Psi(\lambda-\mu,\mu)D(\mu,t)\,v(\lambda-\mu,t)\,d\mu = \int_0^\lambda \Psi(\lambda-\mu,\mu)D(\lambda-\mu,t)\,v(\mu,t)\,d\mu
$$

then (2.27) becomes

$$
\begin{aligned}
\frac{\partial D}{\partial t}(\lambda,t) &= \frac{1}{2}\int_0^\lambda \Psi(\lambda-\mu,\mu)D(\lambda-\mu,t)[u(\mu,t) + v(\mu,t)]\,d\mu \\
&\quad - D(\lambda,t)\int_0^\infty \Psi(\lambda,\mu)u(\mu,t)\,d\mu - v(\lambda,t)\xi(\lambda)\int_0^\infty \xi(\mu)D(\mu,t)\,d\mu \qquad (2.28)
\end{aligned}
$$

Since we have already proved that $Q(t) = \int_0^\infty \xi(\mu)\,D(\mu,t)\,d\mu = 0,\ \forall t \in [0,T]$ for some arbitrary time $T \leq T_b$ then we obtain

$$
\begin{aligned}
\frac{\partial D}{\partial t}(\lambda,t) &= \frac{1}{2}\int_0^\lambda \xi(\lambda-\mu)D(\lambda-\mu,t)\xi(\mu)[u(\mu,t) + v(\mu,t)]\,d\mu \\
&\quad - \xi(\lambda)D(\lambda,t)\int_0^\infty \xi(\mu)u(\mu,t)\,d\mu
\end{aligned}
$$

for any $t \in [0,T]$, with $T \leq T_b$. Moreover, using the previous notations, we can rewrite the equation above in terms of $R(\lambda,t)$ and $P(t)$ as follows:

$$
\frac{\partial R}{\partial t}(\lambda,t) = \frac{\xi(\lambda)}{2}\int_0^\lambda \xi(\mu)R(\lambda-\mu,t)[u(\mu,t) + v(\mu,t)]\,d\mu - \xi(\lambda)R(\lambda,t)P(t) \qquad (2.29)
$$

for any $t \in [0,T]$, with initial condition $R(\lambda,0) = 0$. Equivalently, equation (2.29) can be rewritten as

$$
R(\lambda,t) = \frac{\xi(\lambda)}{2}\int_0^t\int_0^\lambda R(\lambda-\mu,s)\xi(\mu)[u(\mu,s) + v(\mu,s)]\,d\mu\,ds - \xi(\lambda)\int_0^t R(\lambda,s)P(s)\,ds \qquad (2.30)
$$

Since $u(\lambda,t)$, $v(\lambda,t) \geq 0$, $\forall \lambda \geq 0$, $t \in [0,T]$ then we have

$$|R(\lambda,t)| \leq \frac{\xi(\lambda)}{2} \int_0^t \int_0^\lambda |R(\lambda-\mu,s)| \xi(\mu) \left[u(\mu,s)+v(\mu,s)\right] d\mu \, ds$$
$$+ \xi(\lambda) \int_0^t |R(\lambda,s)| P(s) \, ds \tag{2.31}$$

Let us now define

$$m(X,T) := \max_{0\leq\lambda\leq X,\, 0\leq t\leq T} |R(\lambda,t)|$$

Then we obtain the following inequality

$$m(X,T) \leq m(X,T)\,\xi(X) \left\{ \frac{1}{2} \int_0^T \int_0^X \xi(\mu)\left[u(\mu,s)+v(\mu,s)\right] d\mu\, ds + \int_0^T P(s)\, ds \right\} \forall X,T \tag{2.32}$$

If $m(X,T) = 0$ then $R(\lambda,t) = 0$. So, $D(\lambda,t) = 0$ and thus uniqueness of solutions holds, i.e. $u(\lambda,t) = v(\lambda,t)$, for all $0 \leq \lambda \leq X, 0 \leq t \leq T \leq T_b$. Otherwise, if uniqueness fails, then for every $T > 0$, there exists $X \geq 0$ such that $R(X,T) \neq 0$, so $m(X,T) > 0$. For any such X, we divide (2.32) by $m(X,T)$ and (2.32) becomes

$$1 \leq \xi(X) \int_0^T \left\{ \frac{1}{2} \int_0^X \xi(\mu)[u(\mu,s)+v(\mu,s)]\, d\mu + P(s) \right\} ds \tag{2.33}$$

Let

$$A_T := \{X : m(X,T) > 0\} \quad \text{and} \quad X_T := \inf A_T$$

Then, by continuity (2.33) also holds at $X = X_T$, i.e.

$$1 \leq \xi(X_T) \int_0^T \left\{ \frac{1}{2} \int_0^{X_T} \xi(\mu)[u(\mu,s)+v(\mu,s)]\, d\mu + P(s) \right\} ds \tag{2.34}$$

We first show that X_T is an increasing sequence in T. Indeed, if $T_1 \leq T_2$, then

$$m(X,T_1) = \max_{0\leq\lambda\leq X,\, 0\leq t\leq T_1} |R(\lambda,t)| \leq \max_{0\leq\lambda\leq X,\, 0\leq t\leq T_2} |R(\lambda,t)| = m(X,T_2).$$

Therefore, $m(X,T_2) \geq m(X,T_1)$, for all $X \geq 0$, which proves that $m(X,T)$ is an increasing function in T, for all X. Thus, if $\lambda \in A_{T_1}$ then $m(\lambda,T_1) > 0$ and since $m(\lambda,T_2) \geq m(\lambda,T_1) > 0$, for all $\lambda \in [0,X]$ then $m(\lambda,T_2) > 0$ which proves that $\lambda \in A_{T_2}$. Therefore, $A_{T_1} \subseteq A_{T_2}$. So, $X_{T_1} \leq X_{T_2}$ and thus X_T is an increasing sequence.

We may now let $T \to 0^+$ in (2.34) and we get the following contradiction:

$$1 \leq \xi(X_T) \int_0^T \left\{ \frac{1}{2} \int_0^{X_T} \xi(\mu)[u(\mu,s) + v(\mu,s)]\, d\mu + P(s) \right\} ds \to 0 \quad \text{as } T \to 0^+$$

Therefore, $u(\lambda, t) = v(\lambda, t)$ holds for $0 \leq \lambda \leq X$, $0 \leq t \leq T$, for X fixed and T sufficiently small. Since X (though) fixed was arbitrary, this in fact covers all values of $\lambda \geq 0$ as well. Next, we prove the uniqueness holds for all $t \geq 0$. Indeed, let u and v be two solutions to the initial value problem (2.8), (2.9) such that $u(\lambda, 0) = v(\lambda, 0)$. Let us denote by

$$T_0 := \sup \left\{ t \geq 0 \quad \text{s.t.} \quad u(\lambda, \tau) = v(\lambda, \tau), \quad \forall \lambda \geq 0 \quad \text{and} \quad \tau \in [0, t] \right\}$$

Since we have proved that there is a unique solution on some small interval $[0, \tau_0]$, we have $T_0 > 0$. Suppose, $T_0 < \infty$. Then it follows, by continuity of the solutions u and v, that $u(\lambda, T_0) = v(\lambda, T_0)$. Consequently, it results that the following limit

$$P_0(\lambda) := \lim_{t \to T_0^-} u(\lambda, t) = u(\lambda, T_0) = v(\lambda, T_0) \in X_\xi \text{ exists.} \tag{2.35}$$

Therefore, both u and v are solutions to the initial value problem (2.8), (2.9). Since we have proved that local uniqueness of a solution holds, it will result that $u \equiv v$ on some interval $[T_0, T_0 + \tau_0]$ and thus we have a contradiction. Thus, $T_0 = \infty$ as required. Therefore the initial value problem (2.8), (2.35) has a unique non-negative solution for all $t \in [0, \infty)$, and thus the proof of the theorem is now complete. □

Chapter 3

Symmetry methods. Generalities

3.1 Importance of Lie symmetry analysis

Most of the mathematical models used to describe physical problems involve solving differential equations. Although there are a variety of techniques available for obtaining exact solutions to differential equations, most of them can be applied only for a limited class of problems [53]. There are still many open problems that need to be solved, mainly because they are either of a higher order or highly nonlinear.

In the late 19th century, the Norwegian mathematician Sophus Lie developed a remarkable theory that gave rise to a powerful mechanism for solving differential equations. Lie's fundamental discovery was that most of the well-known solution methods, such as the integrating factor, reduction of order, homogeneous or separable solutions, conservation laws, invariant solutions or invertible linear transformations are in fact special cases of a more general integration theory based on the invariance of the equation under a continuous group of symmetry transformations [80].

Lie introduced the notion of a continuous group of transformations in order to deal with the wide variety of techniques for solving ODEs. A symmetry group of a system of differential equations is a group of transformations which maps each of its solutions to another solution of the same system. Of course, there are an infinite number of ways to represent such a mapping by allowing an arbitrary change of independent variables. However, a unique representation occurs if the independent variables are kept fixed. In the classical framework of Lie, these groups depend on continuous parameters and consist of either point transformations (also called classical symmetries) acting on the space of independent and dependent variables or contact transformations acting on the space including all first derivatives of the dependent variables [14].

In most of the cases where exact solutions of differential equations can be obtained, the fundamental property used is the symmetry of that equation. For example, using Lie symmetry analysis one can obtain the ansatz $y(x) = C\,e^{\lambda x}$ for linear homogeneous equations with constant coefficients $y''(x) + a\,y'(x) + b\,y(x) = 0$.

Finding solutions (exact or analytical) to higher order differential equations or nonlinear partial differential equations is one of the most challenging problems in applied mathematics. Lie symmetry methods provide a powerful tool for generating transformations that can be used to reduce the given differential equation into a simpler equation while preserving the invariance of the original equation. When dealing with differential equations for which there is no direct method of solution, we usually look for transformations that either reduce the order of the differential equations (in the case of an ODE) or the number of independent variables (in the case of a PDE), such that the differential equation also remains invariant (unchanged) under these symmetry transformations.

Lie proved that for a given differential equation, a continuous group of point transformations acting on the space of its independent and dependent variables admitted by the equation, can be determined by using a straightforward computational algorithm (Lie's algorithm). Lie's First Fundamental Theorem (2.3.1-1 see e.g. [13]) shows that such Lie symmetry groups are completely characterized by their infinitesimal generators, which form a corresponding Lie algebra under the commutation operator [12, 13, 14, 53, 80, 81]. The functions that appear in the infinitesimal generator of a Lie group of transformations satisfy an overdetermined system of linear differential equations [13]. In the case of point transformations, these functions depend only on the independent and dependent variables. Common examples of such Lie groups of transformations include translations, rotations, and scalings. For instance, an autonomous system of first order differential equations (or a stationary flow) essentially defines a one-parameter Lie group of point transformations [14].

After being determined, the symmetry group of a differential equation has many applications. For example, in some cases one can determine new solutions using the defining property of such a group. Thus, from known solutions one obtains classes of equivalent solutions, where equivalence means that one solution can be obtained by applying a symmetry to a different solution. For example, the heat equation $u_t = u_{xx}$ admits the constant solution $u = C$. From this solution one can derive the fundamental solution $u(x, t) = (4\pi\,t)^{-1/2}\exp(-x^2/4t)$ using only the knowledge of its symmetries. In some other cases, if a system of PDEs is invariant under a Lie group of point transformations, one can find constructively special solutions known as group invariant solutions, or similarity solutions, which are solutions that are invariant under a particular symmetry or some subgroup of the full Lie group admitted by the system. These solutions result from solving a reduced system of differential equations with fewer independent variables. For many nonlinear systems of partial differential equations (which include our PDE in Section 4.2), these types of solutions are the only available and thus they are of great importance. Self-similar solutions are particular similarity solutions which are invariant by some scaling transformation. Similarity solutions are extremely important in Chapter 4 of this thesis, and in general in the symmetry analysis of systems of PDEs or IDEs. These types of solutions may describe the behaviour of general solutions of systems of PDEs or IDEs.

Lie groups and their infinitesimal generators can be naturally extended to act on the space of independent and dependent variables and the derivatives of the dependent variables up to any finite order. Thus the applicability of symmetry methods to differential equations can be extended by considering invariance under the so-called Lie-Bäcklund transformations, whose existence was recognized by E. Noether in 1918 and discussed in detail by Olver [80] and Ibragimov [54]. A very comprehensive reference book containing symmetries of many PDEs is [54].

3.2 Group symmetry methods for partial differential equations

In this section we provide a short summary of the theory of one-parameter Lie groups of point transformations for general partial differential equations with one dependent variable and two independent variables. For a complete study of the general similarity methods see e.g. [12, 13, 14, 18, 53, 54, 69, 80, 81].

Consider a general PDE with two independent variables (x and t) and one dependent variable F of the form

$$\mathcal{R}(x, t, F, F_x, F_t, ...) = 0 \tag{3.1}$$

where the subscripts denote partial differentiation of the dependent variable w.r.t. the independent variables.

Consider a general one-parameter (ε) Lie group of point transformations acting on the independent and dependent variables of the equation (3.1) defined by the equations

$$\begin{aligned} x^* &= \phi(x,t,F;\varepsilon) \\ t^* &= \Psi(x,t,F;\varepsilon) \\ F^* &= \Omega(x,t,F;\varepsilon) \end{aligned} \tag{3.2}$$

where ε is a real parameter that varies over some open interval $|\varepsilon| < \varepsilon_0$ containing zero. Moreover, ϕ, Ψ, and Ω are analytic functions on their respective domains. When $\varepsilon = 0$, the transformation above corresponds to the identical transformation, that is $x^* = x$, $t^* = t$ and $F^* = F$. For a fixed ε, the transformation above is a diffeomorphism that maps the surface (x,t,F) to the surface (x^*,t^*,F^*) parametrized by x and t. In addition, the one-parameter Lie group is assumed to be a local Lie group of transformations (for definition see e.g. [13, 14, 53, 81]).

Definition 2 ***(Symmetry Condition)*** *A partial differential equation (3.1) is called invariant under a local Lie group of point transformations if and only if*

$$\mathcal{R}(x^*,t^*,F^*,F^*_{x^*},F^*_{t^*},...) = 0 \quad \textit{when} \quad \mathcal{R}(x,t,F,F_x,F_t,...) = 0. \tag{3.3}$$

If (3.3) holds, then we say that the point transformation (3.2) is a point symmetry admitted by (3.1). In this case, the Lie group is called a Lie symmetry for the PDE.

Often, the symmetry condition (3.3) for a differential equation is nonlinear and extremely complicated, so we will not attempt to solve (3.3) directly. Lie proved that it is possible to replace this condition with the so-called linearized symmetry condition [53], also called the infinitesimal criterion for the invariance of the PDE (see e.g. [13, 14]).

For this purpose, we consider the infinitesimal generator of the Lie group of point transformations defined by

$$X = \xi(x,t,F)\,\frac{\partial}{\partial x} + \zeta(x,t,F)\,\frac{\partial}{\partial t} + \eta(x,t,F)\,\frac{\partial}{\partial F} \tag{3.4}$$

see e.g. [13, 53, 80], where

$$\xi(x,t,F) \equiv \frac{\partial}{\partial\varepsilon}\phi(x,t,F;0), \quad \zeta(x,t,F) \equiv \frac{\partial}{\partial\varepsilon}\Psi(x,t,F;0), \quad \eta(x,t,F) \equiv \frac{\partial}{\partial\varepsilon}\Omega(x,t,F;0)$$

are called the generators of the Lie group of point transformations. Here, X represents the linear part or the $\mathcal{O}(\varepsilon)$ terms in a Taylor series expansion of the one-parameter

(ε) Lie group of transformations about $\varepsilon = 0$. Thus, we seek for Lie point symmetries of the form

$$\begin{aligned} x^* &= x + \varepsilon\xi(x,t,F) + O(\varepsilon^2) \\ t^* &= t + \varepsilon\zeta(x,t,F) + O(\varepsilon^2) \\ F^* &= F + \varepsilon\eta(x,t,F) + O(\varepsilon^2) \end{aligned} \tag{3.5}$$

In order to derive a condition for the invariance of the PDE (3.1) in terms of the generators of the local Lie group, we expand the left-hand side of the first equation in (3.3) and carry out the differentiation by using the chain rule. For this purpose, we need to consider the prolongation of the point transformation to first derivatives (see e.g. [12, 13, 80])

$$\begin{aligned} F^*_{x^*} &= F_x + \varepsilon\,\eta^x(x,t,F,F_x,F_t) + O(\varepsilon^2) \\ F^*_{t^*} &= F_t + \varepsilon\,\eta^t(x,t,F,F_x,F_t) + O(\varepsilon^2) \end{aligned}$$

where η^x and η^t represent the infinitesimals of $F^*_{x^*}$ and $F^*_{t^*}$ given by

$$\eta^x = \eta_x + (\eta_F - \xi_x)\,F_x - \zeta_x\,F_t - \xi_F\,F_x^2 - \zeta_F\,F_x\,F_t \tag{3.6}$$

$$\eta^t = \eta_t + (\eta_F - \zeta_t)\,F_t - \xi_t\,F_x - \zeta_F\,F_t^2 - \xi_F\,F_x\,F_t \tag{3.7}$$

where the superscripts are function labels. Furthermore, we also consider the prolongation of the infinitesimal generator X to first order derivatives given by [12, 14, 53]:

$$X^{(1)} = \xi\,\frac{\partial}{\partial x} + \zeta\,\frac{\partial}{\partial t} + \eta\,\frac{\partial}{\partial F} + \eta^x\,\frac{\partial}{\partial F_x} + \eta^t\,\frac{\partial}{\partial F_t} \tag{3.8}$$

For higher order PDEs one also needs to consider the prolongation of the Lie group of point transformations and infinitesimal generator X to second, ..., k-th order derivatives. Therefore, we obtain the following invariance condition for the PDE (3.1)

Definition 3 *The one-parameter Lie group of point transformations is a point symmetry of the PDE (3.1) if and only if* $X^{(1)}\mathcal{R} = 0$ *when* $\mathcal{R} = 0$.

More explicitly, using the definition of $X^{(1)}\mathcal{R}$ obtained in (3.8) we have the following

Definition 4 ***(Infinitesimal Criterion for the invariance of the PDE (3.1))*** *The PDE (3.1) is said to be invariant under the Lie group of point transformations if and only if*

$$\xi\,\frac{\partial\mathcal{R}}{\partial x} + \zeta\,\frac{\partial\mathcal{R}}{\partial t} + \eta\,\frac{\partial\mathcal{R}}{\partial F} + \eta^x\,\frac{\partial\mathcal{R}}{\partial F_x} + \eta^t\,\frac{\partial\mathcal{R}}{\partial F_t} = 0. \tag{3.9}$$

The equation (3.9) is called the invariance condition [12, 13, 14, 80, 81] or the linearized symmetry condition [53].

If a solution to the PDE (3.1) is invariant under the group of transformations, then the solution must map into itself, which means $F^*(x^*, t^*) = F(x^*, t^*)$. These types of solutions are also known as similarity solutions. In terms of the transformation functions, the equation above can be written as

$$F(x + \varepsilon\,\xi,\; t + \varepsilon\,\zeta) = F(x,t) + \varepsilon\,\eta(x,t,F) + \mathcal{O}(\varepsilon^2) \tag{3.10}$$

Expanding the left-hand side of the equation (3.10), and equating the coefficients of ε, we obtain the following

Definition 5 *(see e.g. [53]) A surface $F = F(x,t)$ is called invariant under a Lie group of point transformations if and only if the characteristic of the group defined by*

$$Q(x,t,F,F_x,F_t) = \eta(x,t,F) - \xi(x,t,F)\,\frac{\partial F}{\partial x} - \zeta(x,t,F)\,\frac{\partial F}{\partial t}$$

satisfies the so-called ***invariant surface condition****,*

$$Q(x,t,F,F_x,F_t) = 0 \quad \textit{when} \quad F = F(x,t). \tag{3.11}$$

The generated similarity solution satisfies the auxiliary first order partial differential equation (3.11) whose coefficients depend on the infinitesimals of the group.

In order to find the infinitesimal elements (ξ, ζ, η) leaving (3.11) invariant (thus satisfying (3.1)), the original PDE may be used to eliminate one of the derivatives (if possible) and then substitute these in (3.9). The resulting equation is treated as a form in the derivatives of the solution F whose coefficients depend on (x,t,F) and the unknowns (ξ, ζ, η). After the substitution, the remaining terms are split with respect to their dependence on the derivatives of F. Next, we collect together the coefficients of like derivative terms in F and set all of them equal to zero. By doing so, we obtain an overdetermined linear system of so-called determining equations for the generators ξ, ζ, η. Having determined the infinitesimals of the group, we return to the invariant surface condition (3.11). Solving the corresponding characteristic equations of this first order PDE

$$\frac{dx}{\xi(x,t,F)} = \frac{dt}{\zeta(x,t,F)} = \frac{dF}{\eta(x,t,F)}$$

one finds the functional form of the similarity solution, and thus candidates for self-similar solutions. This solution involves two constants, one becomes the independent variable $s(F, x, t)$, called the *similarity variable* and the other is the dependent variable $\psi(s)$, also called the *similarity profile.* Thus, we obtain the *similarity solution* to be

$$F = \mathcal{F}(x, t, s, \psi(s)) \tag{3.12}$$

with the dependence of $\mathcal{F}$ on x, t and the arbitrary function $\psi(s)$ known explicitly. Substitution of (3.12) into (3.1) results in an ordinary differential equation for the function $\psi(s)$. Thus, the invariance under a one-parameter Lie group of point transformations reduces a PDE with two independent variables to an ODE which in general is much easier to solve than the original PDE. After we study the invariance of the PDE, we also analyze the symmetries of the initial and boundary conditions and seek the subalgebra of the infinitesimals leaving invariant the boundary curves and the boundary/initial conditions prescribed on them.

Chapter 4

Application of Lie methods to the coagulation equation

4.1 Self-similar solutions: Previous work

It has been conjectured for several years that Smoluchowski's coagulation equations admit self-similar solutions, also known as scaling invariant solutions. These conjectures have been predicted by physicists Friedlander and Wang [45, 46], van Dongen and Ernst [24], and numerical simulations (Man Hoi Lee [68]) have also confirmed the validity of such assertions. The existence of self-similar solutions though not rigorously justified by physicists, have been mathematically proved in recent years for a few special classes of homogeneous coagulation kernels. It is important to investigate the existence of such special solutions in order to identify their properties for large times $t \to \infty$ and also the behaviour of the size distributions near the gelation time T_{gel}. This approach offers a better understanding of the gelation mechanism which is important in this thesis and for the theory of coagulation in general. The purpose of this section is to provide a brief review of the previous work in the literature with regards to the existence of self-similar solutions to the pure coagulation equations (no particle sources present in the system). Self-similar solutions are interesting particular solutions as they may describe the behaviour of the general solutions of the coagulation equations [24, 35].

There has been lot of scientific interest to study self-similar or dynamical scaling behaviour of the size distribution $c(\lambda, t)$ solution to (2.5) beginning with Friedlander and Wang [46] in 1966 for coagulation by Brownian motion. The authors observed that if the coagulation kernel K is a homogeneous function of degree a, that is

$$K(u\,\lambda, u\,\mu) = u^a\,K(\lambda, \mu), \text{ for some exponent } a, \text{ where } u,\ \lambda,\ \mu > 0,$$

then the transformation (ansatz)

$$\eta = \frac{\lambda}{\xi(t)} \quad \text{and} \quad \xi(t)\, c(\lambda, t) = M_0(t)\, \psi(\eta)$$

reduces the coagulation equation to an ordinary integro-differential equation for $\psi(\eta)$. This solution is called self-preserving solution of the Smoluchowski's coagulation equation. Such a solution $\psi(\eta)$ is an asymptotic solution to which the system is expected to converge, regardless of the initial distribution $c_0(\lambda)$. The authors have obtained this form of the self-preserving solution by solving the coagulation equation numerically up to the point where the size distribution, expressed in the form $\psi(\eta)$, remains fixed with some preset accuracy. Other self-similar solutions have been obtained in [11, 75]. The investigation of the structure of scaling solutions of Smoluchowski's coagulation equation continued in 1988 with the work provided by the physicists van Dongen and Ernst [24]. The authors asserted that the solutions approach a scaling invariant form

$$c(\lambda, t) \ \xrightarrow{S}\ c_S(\lambda, t) = [s(t)]^{-\tau}\, \varphi_\tau(\lambda / s(t)) \tag{4.1}$$

where $\tau > 0$, $s(t)$ represents the average cluster size and $\varphi_\tau(x)$ is a scaling function, also known as the similarity profile, where $x \equiv \lambda/s(t)$. Thus, in the scaling limit, $c_S(\lambda, t)$ becomes independent of the details of the initial distribution. The authors calculated the time dependence of the mean cluster size $s(t)$, and studied the shape of the function $\varphi_\tau(x)$ for different classes of coagulation kernels $K(\lambda, \mu)$. Moreover, they provide formal arguments suggesting that gelation occurs if $a > 1$, and does not occur if $a \leq 1$. Both gelling and nongelling models are characterized by the divergence of the average cluster size $s(t)$ as $t \to T_{gel}$ and $t \to \infty$, respectively. In the gelling and nongelling models, the particle mean size $s(t)$ and the self-similar profile φ_τ need to be determined. These functions depend on the coagulation kernel but not on specific properties of the initial data $c_0(\lambda)$. In the gelling models, it was proved (see e.g. [24]) that $s(t)$ diverges at a finite time as $s(t) \sim (T_{gel} - t)^{-1/\sigma}$, where the critical exponent $\sigma = (a-1)/2$. The value of τ is correct for $a = 2$ (i.e. the multiplicative kernel). Moreover, the scaling function $\varphi_\tau(x)$ falls off algebraically as $x \to 0$ in the form $\varphi_\tau(x) \sim B\, x^{-\tau}$, where the value $\tau = (a+3)/2$ has been proposed. However, numerical simulations performed in [68] seem to indicate a different value for the exponent τ.

The approach to self-similarity (or dynamical scaling) has only been recently established rigorously for the pure coagulation equation ($g \equiv 0$), for a class of solvable and homogeneous kernels $K = 2$, $\lambda + \mu, \lambda \mu$ (see e.g. [57, 75, 76]). For the constant and linear kernels, some explicit examples of self-similar solutions are already known in the literature (see e.g. [35, 75, 76]), as follows: for $K(\lambda, \mu) = 1$, the solution is

$$c(\lambda, t) = 4\, t^{-2}\, e^{-2\lambda/t}, \quad t > 0$$

while for $K(\lambda, \mu) = \lambda + \mu$, the solution is

$$c(\lambda, t) = (2\,\pi)^{-1/2}\, e^{-t}\, \lambda^{-3/2}\, e^{-e^{-2t}\,\lambda/2}$$

For the multiplicative kernel $K(\lambda, \mu) = \lambda\, \mu$ it was shown in [75] that there exists an interval of values for $\tau \in [5/2, 3)$ for which a self-similar solution of the form (4.1) exist. For this particular kernel, the form of $s(t)$ and φ_τ are known explicitly (see e.g. [75]) to be

$$s(t) = (T - t)^{-1/(3-\tau)} \quad \text{and} \quad \varphi_{5/2}(x) = (4\,\pi)^{-1/2}\, x^{-5/2}\, e^{-x/4}, \quad \text{for} \quad \tau = 5/2$$

and, for $\tau \in (5/2, 3)$,

$$\varphi_\tau(x) \sim c_0\, x^{-\tau} \quad \text{as} \quad x \to 0 \quad \text{and} \quad \varphi_\tau(x) \sim c_\infty\, x^{-(2\tau-3)/(\tau-2)} \quad \text{as} \quad x \to \infty$$

for some positive constants c_0, c_∞ and T. Menon and Pego [75, 76] have also considered the approach to self-similarity (or dynamical scaling) of the cluster size distribution for the "solvable" coagulation kernels above. In the case of continuous cluster size distributions, the authors prove the uniform convergence of the size distributions to a self-similar solution with exponential tail. This convergence is proved under the regularity hypothesis that a suitable moment has an integrable Fourier transform.

For general homogeneous kernels with degree of homogeneity $a \in [0, \infty) \setminus \{1\}$, van Dongen et al [24], Escobedo et al. [35], Leyvraz [63], provided some forms of self-similar solutions to the pure coagulation equation, as follows: For $a \in [0, 1)$,

$$c_S(\lambda, t) = t^{-2/(1-a)}\, \psi\Big(\lambda\, t^{-1/(1-a)}\Big)$$

where $\psi(z)$ satisfies the nonlinear ordinary IDE

$$2\,\psi(z) + z\,\psi'(z) + (1 - a)\,\mathcal{C}(\psi)(z) = 0$$

and $\mathcal{C}$ denotes the coagulation operator given by [35]

$$\mathcal{C}(\psi)(z) = \frac{1}{2} \int_0^z K(z - z', z')\,\psi(z - z')\,\psi(z')\,dz' - \psi(z) \int_0^\infty K(z, z')\,\psi(z')\,dz'$$

Furthermore, for $a > 1$,

$$c_S(\lambda, t) = (1-t)^{\alpha}\, \psi(\lambda\,(1-t)^{\beta})$$

where α, β satisfy $\alpha + 1 = \beta\,(1+a)$. The author acknowledges that the case $a > 1$ reduces to solving a non-linear eigenvalue problem for the similarity profile $\psi(z)$. The latter is left as an open problem in [35], however the author refers to a similar related problem for the solution of a linearised Uehling Uhlenbeck equation. Rigorous mathematical proofs for the existence of at least one scaling profile $\psi(z)$ for three classes of homogeneous (nongelling) kernels with degree of homogeneity $a < 1$ have been provided recently by Fournier and Laurençot [43] and Escobedo et al [37].

For more practical coagulation kernels, which include non-homogeneous functions, in a process where particle sources and sinks may be present in the coagulating system, one might be interested in the existence of self-similar solutions. To our knowledge, there are no scaling invariant forms (or self-similar solutions) currently available for the size distributions, as in this case it is not straightforward to predict a general ansatz for the solutions or a scaling form to which these systems could converge. Since self-similar solutions are particular solutions that are invariant by some scaling transformation (see the ansatz (4.1)), our goal is to determine special classes of solutions which possess a type of invariance under more general transformations of the variables, such as: stretchings, rotations, scalings, translations. Hence the self-similar solutions obtained so far in the literature of coagulation are in fact particular examples of similarity solutions. Our main purpose in this thesis is to obtain general similarity solutions using a systematic and practical method based on invariance under continuous Lie groups of transformations as described in Chapter 3. In the next two sections of this chapter we apply the Lie symmetry group methods to derive general similarity solutions for coagulation equations. In Section 4.2 we apply this method to a PDE associated to the coagulation equation with the kernel $K(\lambda, \mu) = (\alpha + \beta\,\lambda)\,(\alpha + \beta\,\mu)$. We call this an *indirect method*. In Section 4.3 we generalize the method in Section 4.2 for PDEs and apply this to the coagulation equation directly with the kernel $K(\lambda, \mu, t) = (\alpha(t) + \beta(t)\,\lambda)\,(\alpha(t) + \beta(t)\,\mu)$. We refer to this as a *direct method*. The theoretical approach we propose in Sections 4.2, 4.3 is presented for a class of coagulation kernels of the form (4.4) and (4.171), respectively. Our methods can be extended to include more general kernels (at least of product type and possibly others) and can also be applied to coagulation-fragmentation equations with sources and sinks or to kinetic equations (specially integro-differential equations).

We obtain a few similarity solutions to the coagulation equation and show that for some special initial conditions these are in fact exact solutions to the original equation (4.2). In some cases we recover previous known explicit solutions for the pure coagulation equations, however we also provide new family of solutions (analytical, formal series and asymptotic) in the presence or absence of sources. Furthermore, using the scaling transformation for the time variable t described in Section 2.1, one can derive then solutions to the original coagulation equation (1.1) with particle sources and sinks.

It is important to obtain similarity (group-invariant) solutions for the coagulation equation as these solutions can be used to derive particular solutions that may describe the behaviour of the general solutions of the coagulation equations. These similarity solutions can be used to provide a study of the asymptotic behaviour of solutions to the coagulation equations for large sizes ($\lambda \to \infty$) and near the gelation point ($t \to T_{gel}$). This asymptotic behaviour of solutions will be further used for numerical purposes in Section 5.3 when dealing with the improper integral there. An analysis of the asymptotic large size behaviour of solutions was provided by Ernst et al. in [34] based on the saddle point method for the inverse Laplace transform. However, the method in [34] relies on a knowledge of the expression of the total mass (first moment of the solution c). The advantage of working with a modified version of the coagulation equation (as in Sections 4.2, 4.3) is that when we develop the general similarity method for these equations the similarity solutions depend on the zeroth and first moments which are determined as solutions of first order differential equations. In some cases it is not straightforward to obtain the solution $c(\lambda, t)$, however as will be shown in Section 5.3, knowledge of the gelation time and the first moment of the solutions are also invaluable.

4.2 Symmetry methods applied to a PDE associated to the coagulation equation

In this section, we provide the group analysis for a quasilinear first order partial differential equation associated to the coagulation equation in the presence of particle source terms. This analysis provides us with a family of similarity solutions or group-invariant solutions for the coagulation equation. In some particular cases we derive explicit solutions $c(\lambda, t)$ and the asymptotic behaviour of solutions to the coagulation equations with particle source terms at large size ($\lambda \to \infty$) for a few special classes of initial conditions and a bilinear, separable coagulation rate (kernel) in the pre- and post- gelation stages. These solutions depend on the first moment of solution $M_1(t)$ which is itself a solution to an ordinary differential equation. In most of the cases we determine explicitly the formula for the total mass for all $t \geq 0$ and also the expression of the gel-time. These similarity solutions can also be used to investigate the size distribution function numerically.

Consider the coagulation equation with particle source terms given by

$$\frac{\partial c}{\partial t}(\lambda, t) = \frac{1}{2}\int_0^\lambda K(\lambda-\mu, \mu)c(\lambda-\mu, t)c(\mu, t)d\mu - c(\lambda, t)\int_0^\infty K(\lambda, \mu)c(\mu, t)d\mu + g(\lambda, t) \tag{4.2}$$

for any λ, $t \geq 0$, subject to initial condition

$$c(\lambda, 0) = c_0(\lambda), \quad \lambda \geq 0. \tag{4.3}$$

In this section, we consider a particular case of coagulation kernel of the form

$$K(\lambda, \mu) = \theta(\lambda)\,\theta(\mu), \quad \text{where} \quad \theta(\lambda) = \alpha + \beta\,\lambda,\ \alpha \geq 0,\ \beta > 0 \text{ arbitrary constants.} \tag{4.4}$$

As described in Chapter 1, the following quantities are important for our study

$$M_k(t) = \int_0^\infty \lambda^k\, c(\lambda, t)\, d\lambda, \quad \text{where} \quad k = 0, 1, 2 \tag{4.5}$$

which represent the k^{th} moment of the solution $c(\lambda, t)$.

Due to the very special form (4.4) of the kernel K, we may use Laplace transforms formally to convert the equation (4.2) to a first order quasilinear PDE. For this purpose, we introduce the following notations:

$$\begin{aligned}
u(x,t) &:= \int_0^\infty e^{-\lambda x}\,\theta(\lambda)\,c(\lambda,t)\,d\lambda = \mathcal{L}\{\theta(\lambda)\,c(\lambda,t)\}(x,t)\\
N(t) &:= \int_0^\infty \theta(\lambda)\,c(\lambda,t)\,d\lambda \quad\Rightarrow\quad u(0,t) = N(t),\ \forall t \geq 0\\
H(x,t) &:= \int_0^\infty e^{-\lambda x}\,\theta(\lambda)\,g(\lambda,t)\,d\lambda = \mathcal{L}\{\theta(\lambda)\,g(\lambda,t)\}(x,t)\\
h(x) &:= \int_0^\infty e^{-\lambda x}\,\theta(\lambda)c_0(\lambda)\,d\lambda = u(x,0) \quad\Rightarrow\quad h(0) = N(0) \qquad (4.6)
\end{aligned}$$

where, as usual $\mathcal{L}\{...\}$ denotes the Laplace transform. The condition $u(0,t) = N(t)$ is called the "compatibility condition" (see e.g. [89]). We begin by eliminating the "infinite integral" from the equation (4.2), in the form of the function $\theta(\lambda)\,N(t)\,c(\lambda,t)$ by means of an integrating factor. To do this, multiply (4.2) by $e^{\theta(\lambda)\,Q(t)}$, where $Q(t) = \int_0^t N(\tau)\,d\tau$ and denote by

$$f(\lambda,t) := e^{\theta(\lambda)\,Q(t)}\,c(\lambda,t) \quad \text{and} \quad p(\lambda,t) := e^{\theta(\lambda)\,Q(t)}\,g(\lambda,t).$$

Then the coagulation equation reduces to the following IDE for $f(\lambda,t)$:

$$\frac{\partial f}{\partial t}(\lambda,t) = \frac{1}{2}\,e^{-\alpha Q(t)} \int_0^\lambda \theta(\lambda-\mu)\,\theta(\mu) f(\lambda-\mu,t)\,f(\mu,t)\,d\mu + p(\lambda,t) \qquad (4.7)$$

subject to initial condition

$$f(\lambda,0) = c(\lambda,0) = c_0(\lambda). \qquad (4.8)$$

Next, define the Laplace transforms of $\theta(\lambda)f(\lambda,t)$ and $\theta(\lambda)p(\lambda,t)$ by

$$\begin{aligned}
F(x,t) &:= \int_0^\infty e^{-\lambda x}\,\theta(\lambda)\,f(\lambda,t)\,d\lambda = \mathcal{L}\{\theta(\lambda)\,f(\lambda,t)\}(x,t) = e^{\alpha Q(t)}\,u(x-\beta\,Q(t),t)\\
G(x,t) &:= \int_0^\infty e^{-\lambda x}\,\theta(\lambda)\,p(\lambda,t)\,d\lambda = \mathcal{L}\{\theta(\lambda)\,p(\lambda,t)\}(x,t) = e^{\alpha Q(t)}\,H(x-\beta\,Q(t),t)
\end{aligned} \qquad (4.9)$$

Multiplying (4.7) by $\theta(\lambda)$ and formally taking the Laplace transform, we obtain the following PDE for the transformed variable $F(x,t)$:

$$\frac{\partial F}{\partial t}(x,t)\,e^{\alpha Q(t)} + \beta\,F(x,t)\,\frac{\partial F}{\partial x}(x,t) = \frac{\alpha}{2}\,F^2(x,t) + e^{\alpha Q(t)}\,G(x,t),$$
$$(\text{for } x > \beta\,Q(t),\ t \geq 0) \qquad (4.10)$$

subject to the initial condition

$$F(x,0) = h(x) \geq 0, \quad \text{where} \quad x > 0 \tag{4.11}$$

and the compatibility condition

$$F(\beta\, Q(t), t) = Q'(t)\, e^{\alpha\, Q(t)}, \quad t \geq 0 \tag{4.12}$$

where $Q'(t)$ denotes the derivative of $Q(t)$ with respect to t. The equation (4.12) is derived from the first equation in (4.9) by substituting $x = \beta\, Q(t)$ and using the compatibility condition. The initial boundary value problem (IBVP) (4.10-4.12) is not a standard one since the PDE (4.10) has coefficients that are not completely known functions, such as $Q(t)$, which depends on $N(t)$ and thus must be determined as part of the solution [89]. Moreover, the domain of the IBVP is time dependent i.e.

$$\text{Domain IBVP} = \bigcup_{t\geq 0} (\beta\, Q(t), \infty) \times \{t\}.$$

In this section, we present the classical point group analysis of the PDE (4.10) that is based on the classical technique for investigating Lie symmetry groups of differential equations as described in Section 3.2. Such a group analysis provides similarity solutions to PDEs and systems of PDEs containing an arbitrary number of dependent and independent variables by reducing the original system to a system with a reduced number of independent variables, see e.g. the reference books [12, 14, 18, 53, 69, 80, 81].

4.2.1 Determining equations for a PDE associated to coagulation equation

Consider the first order PDE (4.10) with the independent variables x, t and the dependent variable F written as a differential function

$$\mathcal{R}(x, t, F, F_x, F_t) := e^{\alpha\, Q(t)}\, F_t + \beta\, F_x\, F - \frac{\alpha}{2}\, F^2 - e^{\alpha\, Q(t)}\, G(x,t) = 0. \tag{4.13}$$

Since the group symmetry method is independent of the initial and boundary conditions, we disregard for the moment these conditions and concentrate only on the new form of the PDE (4.13). We will take these conditions into account when we have determined the form of the similarity solution $f(\lambda, t)$ to provide explicit (analytic) or asymptotic ($\lambda \to \infty$) behaviour of the solutions f and thus of solutions c and also the functions $Q(t)$ and $N(t)$.

As described in Section 3.1, we look for a Lie group of point symmetries of the form (3.5) under which the PDE (4.13) is left invariant. This reduces to solving the invariance condition (3.9) which in this case takes the following form

$$\begin{aligned} -\xi e^{\alpha Q(t)} G_x + \zeta e^{\alpha Q(t)} \big(\alpha Q'(t) F_t - \alpha Q'(t) G - G_t\big) + \eta\big(\beta F_x - \alpha F\big) \\ + \eta^x \beta F + \eta^t e^{\alpha Q(t)} = 0 \end{aligned}$$

To find the Lie point symmetries (3.5), we need to use first the expressions of the infinitesimals η^x and η^t given by (3.6), (3.7) to obtain

$$\begin{aligned} -\xi\, e^{\alpha Q(t)}\, G_x + \alpha\, \zeta\, Q'(t)\, e^{\alpha Q(t)}\, (F_t - G) - \zeta\, e^{\alpha Q(t)}\, G_t + \eta\, (\beta\, F_x - \alpha\, F) \\ + \beta\, F\, \left[\eta_x + (\eta_F - \xi_x)\, F_x - \zeta_x\, F_t - \xi_F\, F_x^2 - \zeta_F\, F_x\, F_t\right] \\ + e^{\alpha Q(t)} \left[\eta_t + (\eta_F - \zeta_t)\, F_t - \xi_t\, F_x - \xi_F\, F_x\, F_t - \zeta_F\, F_t^2\right] = 0. \end{aligned} \tag{4.14}$$

In general, the invariance condition (3.9) contains enough information to determine the unknown infinitesimals (ξ, ζ, η) for a given PDE. We present below a strategy for determining the infinitesimals for the PDE (4.13). We apply the basic Lie algorithm to solve the linearized symmetry (invariance) condition (4.14) as follows (see e.g. [18, 53]):

Step 1. First, identify the terms in the invariance condition (4.14) that are multiplied by the highest powers of the highest derivatives of F. These terms will give some of the determining equations which should be solved first. In our case, we start by equating the terms F_x^2 and F_t^2 to zero. Based on the F_x^2 terms we obtain $\xi_F = 0$ and thus we have $\xi = \xi(x,t)$. Also, from F_t^2 terms we get $\zeta_F = 0$, so $\zeta = \zeta(x,t)$. We use these results to simplify the remaining terms in the linearized symmetry condition (4.14).

Step 2. Next, write down the terms that are multiplied by the highest remaining powers of the highest remaining derivatives in (4.14). The new resulting determining equations become

$$\begin{aligned} & -\xi\, e^{\alpha Q(t)}\, G_x + \alpha\, \zeta\, Q'(t)\, e^{\alpha Q(t)}\, (F_t - G) - \zeta\, e^{\alpha Q(t)}\, G_t + \eta\, (\beta\, F_x - \alpha\, F) \\ & + \beta\, F\, \left[\eta_x + (\eta_F - \xi_x)\, F_x - \zeta_x\, F_t\right] + e^{\alpha Q(t)} \left[\eta_t + (\eta_F - \zeta_t)\, F_t - \xi_t\, F_x\right] = 0 \end{aligned}$$

Step 3. Using the original PDE (4.13) we can eliminate F_t. Substitute, $F_t = -\beta\, e^{-\alpha Q(t)}\, F\, F_x + \frac{\alpha}{2}\, e^{-\alpha Q(t)}\, F^2 + G$ into (4.14).

Step 4. Split the terms according to their dependence on the derivatives of F, i.e. F_x and the remaining terms. We obtain the following linear system of determining equations of the group for the infinitesimal generators ξ, ζ, η:

$$-\alpha\beta Q'(t)\zeta\, F + \beta\eta - \beta\, F\, \xi_x + \beta^2\, e^{-\alpha Q(t)}\, \zeta_x\, F^2 - e^{\alpha Q(t)}\, \xi_t + \beta\, \zeta_t\, F = 0 \quad (4.15)$$

$$\begin{aligned} &- e^{\alpha Q(t)}\, \xi\, G_x + \frac{\alpha^2}{2}\, \zeta\, Q'(t)\, F^2 - \zeta e^{\alpha Q(t)}\, G_t - \alpha\eta\, F + \beta\, F\, \eta_x - \frac{\alpha\,\beta}{2}\, \zeta_x\, e^{-\alpha Q(t)}\, F^3 \\ &- \beta\zeta_x\, G\, F + e^{\alpha Q(t)}\, \eta_t + \frac{\alpha}{2}\, \eta_F\, F^2 - \frac{\alpha}{2}\, \zeta_t\, F^2 + e^{\alpha Q(t)}\, G\, \eta_F - G\, e^{\alpha Q(t)}\, \zeta_t = 0 \end{aligned} \quad (4.16)$$

where $\zeta = \zeta(x, t)$, $\xi = \xi(x, t)$ and $\eta = \eta(x, t, F)$.

The result of the steps above is usually an overdetermined system of linear PDEs in the unknown infinitesimals $(\xi,\ \zeta,\ \eta)$.

To verify the determining equations (4.15), (4.16) above we have also used a software package called **MathLie** provided by G. Baumann [10] and implemented in **Mathematica**. First, we call the function **DeterminingEquations** to generate the determining equations of the group.

```
>> EQ = {[D[F[x,t],t] * Exp[a * Q[t]] + b * F[x,t] * D[F[x,t],x]
- a * F[x,t].^2/2 - Exp[a * Q[t]] * G[x,t]}; EQ//LTF
>> DETEQ = DeterminingEquations[EQ, {F}, {x,t}, {D[F[x,t],t]}]; DETEQ//LTF
```

Using equation (4.15) we can determine the infinitesimal η as

$$\eta(x, t, F) = A\, F^2 + B\, F + C$$

where, for simplicity we denote by

$$A := -\beta\, e^{-\alpha Q(t)}\, \zeta_x, \quad B := \alpha\, Q'(t)\zeta + \xi_x - \zeta_t, \quad \text{and} \quad C := \frac{1}{\beta}\, e^{\alpha Q(t)}\, \xi_t \qquad (4.17)$$

with A, B, C functions of x, and t. Substituting η together with the derivatives

$$\eta_x = A_x\, F^2 + B_x\, F + C_x, \quad \eta_t = A_t\, F^2 + B_t\, F + C_t, \quad \eta_F = 2\, A\, F + B$$

into (4.16) and gathering like powers of F we obtain

$$\begin{aligned}\left(\frac{\alpha}{2}A+\beta A_x\right)F^3+\left[\frac{\alpha^2\zeta}{2}Q'(t)-\alpha B+\beta B_x+e^{\alpha Q(t)}A_t+\frac{\alpha}{2}B-\frac{\alpha}{2}\zeta_t\right]F^2\\ +\left[\beta C_x-\alpha C-\beta\zeta_x G+e^{\alpha Q(t)}B_t+2\,e^{\alpha Q(t)}AG\right]F\\ +e^{\alpha Q(t)}\left[-G_x\xi-G_t\zeta+C_t+BG-G\zeta_t\right]=0\end{aligned}\qquad(4.18)$$

Since the coefficients of the algebraic equation (4.18) are independent of F and F is arbitrary, we obtain the following system of determining equations

$$\frac{\alpha}{2}A+\beta A_x=0 \qquad (4.19)$$

$$\frac{\alpha^2\zeta}{2}Q'(t)-\frac{\alpha}{2}B-\frac{\alpha}{2}\zeta_t+\beta B_x+e^{\alpha Q(t)}A_t=0 \qquad (4.20)$$

$$\beta C_x-\alpha C-\beta\zeta_x G+B_t\,e^{\alpha Q(t)}+2\,AG\,e^{\alpha Q(t)}=0 \qquad (4.21)$$

$$G_x\xi+G_t\zeta+G(\zeta_t-B)-C_t=0 \qquad (4.22)$$

From (4.19) we obtain $A(x,t)=F_1(t)\,e^{-\frac{\alpha}{2\beta}x}$, where $F_1(t)$ is an arbitrary function of t. To determine $B(x,t)$ we need to solve for the infinitesimal $\zeta(x,t)$ first. Based on the definition of $A(x,t)$ we have $\zeta_x(x,t)=-\frac{1}{\beta}\,A(x,t)\,e^{\alpha Q(t)}$.

At this point, in order to determine $\zeta(x,t)$ and the remaining unknown functions B, C and ξ, η we need to consider two separate cases for the constant α, i.e. $\alpha=0$ (thus the kernel is $K(\lambda,\mu)=\lambda\,\mu$) and $\alpha>0$, (so the kernel is $K(\lambda,\mu)=(\alpha+\beta\,\lambda)\,(\alpha+\beta\,\mu)$), where in both cases we have $G(x,t)\geq 0$.

Coagulation kernel $K(\lambda,\mu)=\lambda\,\mu$ and $g(\lambda,t)\geq 0$

This case corresponds to the case when $\alpha=0$ and $G(x,t)\geq 0$. In this subsection, we consider $\beta=1$ as one can rescale the space and time variables in the PDE (4.13). The system (4.19-4.22) takes the form

$$A_x=0 \quad\Rightarrow\quad \zeta_{xx}=0 \qquad (4.23)$$

$$B_x+A_t=0 \quad\Rightarrow\quad \xi_{xx}-2\,\zeta_{xt}=0 \qquad (4.24)$$

$$2\xi_{xt}-\zeta_{tt}-3\,\zeta_x G=0 \qquad (4.25)$$

$$G_x\xi+G_t\zeta+(2\,\zeta_t-\xi_x)\,G=\xi_{tt} \qquad (4.26)$$

$$\eta(x,t,F)=-\zeta_x F^2+(\xi_x-\zeta_t)\,F+\xi_t \qquad (4.27)$$

From $\zeta_{xx}=0$ we obtain $\zeta(x,t)=\zeta_0(t)\,x+\zeta_1(t)$, where $\zeta_0(t)$ and $\zeta_1(t)$ are arbitrary functions of t. Using (4.24) we have $\xi_{xx}(x,t)=2\,\zeta_0'(t)$, so $\xi(x,t)=\zeta_0'(t)\,x^2+\xi_0(t)\,x+$

$\xi_1(t)$, where the coefficients $\xi_0(t)$ and $\xi_1(t)$ are arbitrary functions of t. Substituting $\xi(x,t)$ and $\zeta(x,t)$ into (4.25) we obtain

$$3\,\zeta_0''(t)\,x + 2\,\xi_0'(t) - \zeta_1''(t) = 3\,\zeta_0(t)\,G(x,t). \tag{4.28}$$

Fix $t \geq 0$, and let $x \to \infty$ in (4.28). Then the right-hand side of (4.28) tends to zero. Therefore, we must have $\zeta_0''(t) = 0$ and $2\,\xi_0'(t) - \zeta_1''(t) = 0$, for all t. Since we have assumed that ζ_0 is differentiable, then we have $\zeta_0(t) = a\,t + b$, for some constants a and b. Moreover, $\zeta_0(t)\,G(x,t) = 0$, for all x, t. Therefore the two cases are:

(a) $\zeta_0(t)$ not identically zero. Thus, $G(x,t)$ is identically zero for all x, t.

(b) $\zeta_0(t) = 0$ is identically zero.

In view of the previous analysis, we consider the two subcases above as follows: see Section 4.2.2: $G(x,t) = 0$ (i.e. no sources) and Section 4.2.3: $G(x,t) > 0$ (i.e. sources) below, where in both cases we have $\alpha = 0$.

Coagulation kernel $K(\lambda,\mu) = (\alpha + \beta\,\lambda)\,(\alpha + \beta\,\mu)$ and $g(\lambda,t) \geq 0$

In this case, from (4.19) and using the definition of $A(x,t)$ in (4.17), we obtain

$$A(x,t) = F_1(t)\,e^{-\frac{\alpha}{2\beta}x} \quad \text{and} \quad \zeta(x,t) = \frac{2}{\alpha}\,F_1(t)\,e^{-\frac{\alpha}{2\beta}x}\,e^{\alpha Q(t)} + F_2(t) \tag{4.29}$$

where $F_1(t)$ and $F_2(t)$ are arbitrary functions of t. Using (4.20) and the definition of $A(x,t)$ and $B(x,t)$ in (4.17), we obtain (after integration w.r.t. x)

$$B(x,t) = \frac{\alpha}{2\,\beta}\,e^{\frac{\alpha}{2\beta}x}\,F_4(t) - (F_2'(t) - \alpha\,Q'(t)\,F_2(t)) \tag{4.30}$$

$$\xi(x,t) = -\frac{4\,\beta}{\alpha^2}\,e^{-\frac{\alpha}{2\beta}x}\,e^{\alpha\,Q(t)}\,F_1'(t) + F_4(t)\,e^{\frac{\alpha}{2\beta}x} - \frac{2\beta}{\alpha}\Big(F_2'(t) - \alpha\,Q'(t)\,F_2(t) + \frac{F_3(t)}{\beta}\Big) \tag{4.31}$$

$$\begin{aligned} C(x,t) = &-\frac{4}{\alpha}\,e^{2\alpha Q(t)}\,Q'(t)\,F_1'(t)\,e^{-\frac{\alpha}{2\beta}x} - \frac{4}{\alpha^2}\,e^{2\alpha Q(t)}\,F_1'''(t)\,e^{-\frac{\alpha}{2\beta}x} \\ &+ \frac{1}{\beta}\,e^{\alpha Q(t)}\,F_4'(t)\,e^{\frac{\alpha}{2\beta}x} - \frac{2}{\alpha}\,e^{\alpha Q(t)}\,\Big(F_2''(t) - \alpha\,Q''(t)\,F_2(t) - \alpha\,Q'(t)\,F_2'(t) + \frac{F_3'(t)}{\beta}\Big) \end{aligned} \tag{4.32}$$

where $F_3(t)$ and $F_4(t)$ are arbitrary functions of t. Furthermore, using (4.21) which is equivalent to $\beta\,C_x - \alpha\,C + B_t\,e^{\alpha Q(t)} = -3\,A\,G\,e^{\alpha Q(t)}$ and the formulas above we obtain

$$\left\{2\,e^{\alpha Q(t)}\,Q'(t)\,F_1'(t)+\frac{2}{\alpha}\,e^{\alpha Q(t)}\,F_1''(t)\right\}$$
$$+\frac{1}{3}\,e^{\frac{\alpha}{2\beta}x}\left\{F_2''(t)-\alpha\,Q''(t)\,F_2(t)-\alpha\,Q'(t)\,F_2'(t)+\frac{2\,F_3'(t)}{\beta}\right\}=-F_1(t)\,G(x,t) \tag{4.33}$$

Equation (4.33) suggests that we have to consider two separate cases for $G(x,t)$. Since $G(x,t) \to 0$ as $x \to \infty$ (recall it is expected to be a Laplace transform), we may let $x \to \infty$ in (4.33) to realize that necessarily we have

$$p_1(t) := 2\,e^{\alpha Q(t)}\,Q'(t)\,F_1'(t)+\frac{2}{\alpha}\,e^{\alpha Q(t)}\,F_1''(t)$$
$$p_2(t) := F_2''(t)-\alpha\,Q''(t)\,F_2(t)-\alpha\,Q'(t)\,F_2'(t)+\frac{2\,F_3'(t)}{\beta}$$

Inserting these back in (4.33) leads to $F_1(t)\,G(x,t) = 0$ and thus we consider two separate cases for $G(x,t)$: either $G(x,t) > 0$ which implies $F_1(t) = 0$ or $G(x,t) = 0$. We take each of the cases above and detail them separately as two Subsections 4.2.4 and 4.2.5.

4.2.2 Coagulation kernel $K(\lambda,\mu) = \lambda\mu$ and $g(\lambda,t) = 0$ (no sources)

In this case, we have $\alpha = 0$ and $G(x,t) = 0$, so the PDE (4.13) reduces to the well-known inviscid Burgers' equation

$$F_t(x,t)+F(x,t)\,F_x(x,t)=0. \tag{4.34}$$

Generators for the one-group of transformations

The system of determining equations for the generators reduces to the following equations

$$\zeta_{xx}=0 \quad\Rightarrow\quad \zeta(x,t)=(at+b)\,x+\zeta_1(t) \tag{4.35}$$
$$\xi_{tt}=0 \quad\Rightarrow\quad \xi(x,t)=\xi_2(x)\,t+\xi_3(x) \tag{4.36}$$
$$\xi_{xx}=2\,\zeta_{xt} \quad\Rightarrow\quad \xi_2''(x)\,t+\xi_3''(x)-2\,a=0 \tag{4.37}$$
$$2\,\xi_{xt}=\zeta_{tt} \quad\Rightarrow\quad 2\,\xi_2'(x)=\zeta_1''(t) \tag{4.38}$$
$$\eta=-\zeta_x\,F^2+(\xi_x-\zeta_t)\,F+\xi_t \tag{4.39}$$

(4.38) is possible only if they are both equal to an arbitrary constant c. This means that, $\xi_2''(x) = 0$ and thus $\xi_2'(x) = c$. Also, (4.37) yields $\xi_3''(x) = 2\,a$. Finally, (4.38) implies that $2\,\xi_2'(x) = \zeta_1''(t) = 2\,c$, for some constant c. Thus, with a change in notation we obtain $\zeta_0(t) = a_5 + a_6\,t$, $\zeta_1(t) = a_1 + a_4\,t + a_8\,t^2$, $\xi_2(x) = a_7 + a_8\,x$, and $\xi_3(x) = a_2 + a_3\,x + a_6\,x^2$, where $a_1, ..., a_8$ are arbitrary constants.

Therefore, the generators of the one-group of point transformations that leave the PDE (4.34) invariant take the following form

$$\begin{aligned}
\xi(x,t) &= a_8\,x\,t + a_7\,t + a_6\,x^2 + a_3\,x + a_2 \\
\zeta(x,t) &= a_6\,x\,t + a_5\,x + a_8\,t^2 + a_4\,t + a_1 \\
\eta(x,t,F) &= -(a_6\,t + a_5)\,F^2 + \big(a_6\,x - a_8\,t + a_3 - a_4\big)\,F + a_8\,x + a_7
\end{aligned} \tag{4.40}$$

The infinitesimal generator X associated with the above Lie group of point-transformations can be written as

$$\begin{aligned}
X = {} & a_1\,\frac{\partial}{\partial t} + a_2\,\frac{\partial}{\partial x} + a_3\left(x\,\frac{\partial}{\partial x} + F\,\frac{\partial}{\partial F}\right) + a_4\left(t\,\frac{\partial}{\partial t} - F\,\frac{\partial}{\partial F}\right) + a_5\left(x\,\frac{\partial}{\partial t} - F^2\,\frac{\partial}{\partial F}\right) \\
& + a_6\left(x^2\,\frac{\partial}{\partial x} + x\,t\,\frac{\partial}{\partial t} + (xF - tF^2)\,\frac{\partial}{\partial F}\right) + a_7\left(t\,\frac{\partial}{\partial x} + \frac{\partial}{\partial F}\right) \\
& + a_8\left(x\,t\,\frac{\partial}{\partial x} + t^2\,\frac{\partial}{\partial t} + (x - tF)\,\frac{\partial}{\partial F}\right).
\end{aligned}$$

Therefore, the inviscid Burgers' equation (4.34) has an eight-parameter Lie group of point transformations. More precisely, the infinitesimal symmetry group of (4.34) is spanned by the following eight Lie symmetry vector fields $V_1, V_2, ..., V_8$:

$$\begin{aligned}
& V_1 = \frac{\partial}{\partial t}, \quad V_2 = \frac{\partial}{\partial x}, \quad V_3 = x\,\frac{\partial}{\partial x} + F\,\frac{\partial}{\partial F}, \quad V_4 = t\,\frac{\partial}{\partial t} - F\,\frac{\partial}{\partial F}, \quad V_5 = x\,\frac{\partial}{\partial t} - F^2\,\frac{\partial}{\partial F}, \\
& V_6 = x^2\,\frac{\partial}{\partial x} + x\,t\,\frac{\partial}{\partial t} + (xF - tF^2)\,\frac{\partial}{\partial F}, \quad V_7 = t\,\frac{\partial}{\partial x} + \frac{\partial}{\partial F}, \quad \text{and} \\
& V_8 = x\,t\,\frac{\partial}{\partial x} + t^2\,\frac{\partial}{\partial t} + (x - tF)\,\frac{\partial}{\partial F}
\end{aligned} \tag{4.41}$$

which generate an eight-dimensional Lie algebra L_8. We note that, V_1, V_2 generate translations in t and x directions, respectively; V_5 represents a Galilean transformation in the x direction or a kind of "Galilean boost" to a moving coordinate frame (see e.g. [80]), V_7 generates the rotation in space followed by a translation in the F direction; V_3, V_4 are scalings; and V_6, V_8 are some local groups of transformations. The symmetry groups generated by V_1 and V_2 demonstrate the time- and space- invariance of the equation. The Galilean group generated by V_5 is in fact a product of a translation $F^* = F - \varepsilon\,F^2$ and a "boost" $t^* = t + \varepsilon x$.

These operators form a basis for the corresponding Lie algebra L_8. The Lie algebra is defined by a skew-symmetric bilinear operation, named the Lie bracket (commutator). The commutator of any two vector fields V_i and V_j, is a first order operator defined by

$$[V_i, V_j] = V_i V_j - V_j V_i \qquad \text{(see e.g. [13, 80, 81]).} \tag{4.42}$$

The commutator table for the Lie algebra arising from the infinitesimal generators V_i, where $i = 1, 2, ..., 8$ is presented in Table 4.1. To compute the commutator between two vector fields we used a package called **tensor** in Maple, calling the functions **create; commutator; coord** within this package.

$[V_i, V_j]$	V_1	V_2	V_3	V_4	V_5	V_6	V_7	V_8
V_1	0	0	0	V_1	0	V_5	V_2	$V_3 + 2V_4$
V_2	0	0	V_2	0	V_1	$2V_3 + V_4$	0	V_7
V_3	0	$-V_2$	0	0	V_5	V_6	$-V_7$	0
V_4	$-V_1$	0	0	0	$-V_5$	0	V_7	V_8
V_5	0	$-V_1$	$-V_5$	V_5	0	0	$V_3 - V_4$	V_6
V_6	$-V_5$	$-2V_3 - V_4$	$-V_6$	0	0	0	$-V_8$	0
V_7	$-V_2$	0	V_7	$-V_7$	$V_4 - V_3$	V_8	0	0
V_8	$-V_3 - 2V_4$	$-V_7$	0	$-V_8$	$-V_6$	0	0	0

Table 4.1: Commutator $[V_i, V_j]$ table for the Lie algebra L_8 spanned by V_i and V_j.

From this table it can be seen that V_1 and V_6 generate V_5, V_2 and V_5 generate V_1, etc. So, for example, invariance under translation in x (operator V_2) and under the Galilean transformation (operator V_5) implies invariance under translation in t (operator V_1). It is worth mentioning that several of the groups in the commutator Table 4.1 can be deduced by inspection, particularly invariance under translation of the independent variables (operators V_1 and V_2), or scaling of the dependent and independent variables (operators V_3 and V_4). However, operators such as V_6 and V_8 cannot be found by inspection.

In general, if a PDE (or a differential equation) admits a Lie algebra L_r of dimension $r > 1$, one could in principle consider invariant solutions based on one, two, etc, dimensional subalgebras of L_r [54]. However, there are an infinite number of subalgebras of L_r, for example one-dimensional subalgebras. This problem becomes manageable by recognizing that if two subalgebras are similar, i.e. they are connected with each other by a transformation from the symmetry group (with Lie algebra L_r), then their corresponding invariant solutions are connected with each other by the same transformation. Therefore, it is sufficient to put into one class all similar subalgebras of a given dimension, say s, and select a representative from each class. The set of these representatives of all these classes is called an *optimal system of order s* [54]. In order to find all invariant solutions with respect to s-dimensional subalgebras, it is sufficient to construct invariant solutions for the optimal system of order s. The set of invariant solutions obtained in this way is called an *optimal system of invariant solutions.* The optimal system is determined to ensure that a minimal complete set of reductions of variables is obtained from the symmetries of the given equations. Of course, the form of these invariant solutions depends on the choice of representatives.

In the following we investigate the subalgebra structure (4.41) of the PDE (4.34). In particular, we are interested in determining the optimal system of one-dimensional subalgebras of (4.34) and the corresponding invariant solutions.

For this purpose, we investigate the one-parameter group of adjoint transformations of the one-parameter subgroup $\exp(\varepsilon\, V_i)$ generated by the vector field V_i acting on the vector field V_j, where $i, j = 1, ..., 8$. This representation is denoted by $Ad(\exp(\varepsilon\, V_i))\, V_j$ and is given by the Lie series

$$Ad(\exp(\varepsilon\, V_i))\, V_j = V_j - \varepsilon\, [V_i, V_j] + \frac{\varepsilon^2}{2}\, [V_i, [V_i, V_j]] - ... \tag{4.43}$$

where $[\cdot, \cdot]$ is the usual Lie bracket, defined by (4.42) (see the reference books of Olver [80], and Ovsiannikov [81], for the detailed information for adjoint representation and an optimal system). The corresponding adjoint representation structure for (4.41) can be easily constructed by using the formula (4.43) based on the infinitesimal generators given in the Table 4.1. The resulting operators are given in Table 7.1 in Chapter 7, where each (i, j)-th entry indicates $Ad(\exp(\varepsilon\, V_i))\, V_j$. We adopt the method suggested by Olver [80] to obtain the optimal system of subalgebras for the inviscid Burgers' equation (4.34). We obtain the following result (the proof of Theorem 4.1 is included in Chapter 7).

Theorem 4.1 *A one-dimensional optimal system of one-dimensional subalgebras of the full symmetry algebras for the inviscid Burgers' equation (4.34) is given by the* *following vector fields*

(*i*) $V_8 + V_5 + a_2 V_2 + a_1 V_1$, $V_8 + V_3 + a_2 V_2 + a_1 V_1$, $V_8 \pm V_1$, $V_8 + a_2 V_2$;

(*ii*) $V_7 + V_5 + a_4 V_4$, $V_7 + a_4 V_4 + a_1 V_1$, $V_7 + V_6 + a_4 V_4 + a_1 V_1$;

(*iii*) $V_6 + V_3 + a_2 V_2 + a_1 V_1$, $V_6 + a_1 V_1$, $V_6 + a_2 V_2$;

(*iv*) $V_5 + V_4 + a_3 V_3 + a_2 V_2$, $V_5 + a_3 V_3 + a_2 V_2$;

(*v*) $V_4 + a_3 V_3 + a_2 V_2$, $V_4 + a_3 V_3$, $V_4 + a_2 V_2$;

(*vi*) $V_3 + a_1 V_1$;

(*vii*) $V_2 + a_1 V_1$;

(*viii*) V_1,

where $a_1, a_2, a_3, a_4 \in \mathbb{R}$ *are any real numbers.*

Symmetry reductions for the inviscid Burgers' equation

In this section we present some examples of exact invariant solutions to (4.34) as technical applications. In the theory of Lie groups, if a partial differential equation (or a system) is invariant under a Lie group of point transformations, then some special solutions of these equations can be found. These solutions are called group invariant or similarity solutions, and can be obtained from the solutions of the reduced system of the differential equations with fewer independent variables as described in Chapter 3.

Next, we present the reduction forms of the inviscid Burgers' equations (4.34) by using the corresponding symmetry groups based on the classification of subalgebras in the Theorem 4.1. According to the optimal system of one-dimensional subalgebras of the full symmetry algebras of (4.34), it is possible to obtain the classification of all possible corresponding reduced forms of (4.34).

For illustrating the method in detail, we start by considering the one-dimensional subalgebra spanned by the infinitesimal generator $V_4 + a_3 V_3 + a_2 V_2 + a_1 V_1$ in the *case (v)* of Theorem 4.1, where we have also included the translational symmetry vector V_1. In this case, we obtain invariant solutions to (4.34), by using the so-called *invariant form method* (see e.g. [12, 13, 14]). In some cases we obtain exact invariant solutions to (4.34) and thus explicit (analytic) solutions to the coagulation equation

(4.2). In other cases, we obtain the asymptotic large-size behaviour for the solution $c(\lambda, t)$ of (4.2).

Case I: Vector field $V = V_4 + a_3 V_3 + a_2 V_2 + a_1 V_1$

In this case, the generators of the one-parameter group of transformations that leave the PDE (4.34) invariant are given by

$$\xi(x,t) = a_3 x + a_2, \quad \zeta(x,t) = t + a_1, \quad \eta(x,t,F) = (a_3 - 1) F, \tag{4.44}$$

where a_2, $a_3 \neq 0$ and $a_3 \neq 1$. The case $a_3 = 1$ is not of interest since it leads to a solution $F(x,t) = \frac{x+a_2}{t+a_1}$ which is not completely monotonic.
To obtain invariant solutions one needs to solve the invariant surface condition given by

$$\xi(x,t) F_x + \zeta(x,t) F_t = \eta(x,t,F) \tag{4.45}$$

The equation (4.45) is a first order partial differential equation and it can be solved by the method of characteristics. The characteristic system is given by

$$\frac{dx}{\xi(x,t)} = \frac{dt}{\zeta(x,t)} = \frac{dF}{\eta(x,t,F)}$$

Integrating the first pair of equations gives the first integral (or invariant)

$$s \equiv s(x,t) = \text{constant}.$$

This is the similarity variable (or the independent variable). Letting $x = X(s,t)$ then the second pair becomes:

$$\frac{dt}{\zeta(X(s,t),t)} = \frac{dF}{\eta(X(s,t),t,F)}$$

which can be integrated to obtain another first integral $\omega(s,t,F) = \text{constant}$. This equation determines F which is the similarity solution in terms of s. In principle, the general solution of equation (4.45) can be found. It involves two constants, one becoming the independent variable $s \equiv s(x,t)$ and the other the dependent variable $\psi(s)$. Consequently, we obtain the general similarity solution of (4.45) in the form $F = \mathcal{F}(x,t,s,\psi(s))$ with the dependence of $\mathcal{F}$ on x, t and the arbitrary function $\psi(s)$ known explicitly, as one substitutes F into the original equation and obtains an

ODE for $\psi(s)$. Therefore, we obtain the similarity solutions F and thus candidates for self-similar solutions.

We now return to equation (4.45), where by using the generators (4.44), the invariant surface condition reads as

$$(a_3\, x + a_2)\, F_x + (t + a_1)\, F_t = (a_3 - 1)\, F. \tag{4.46}$$

The system of characteristic equations for (4.46) is given by

$$\frac{dx}{a_3\, x + a_2} = \frac{dt}{t + a_1} = \frac{dF}{(a_3 - 1)\, F} \tag{4.47}$$

For simplicity, we let $a := a_2/a_3 \neq 0$ and $q := a_1$, where q is any constant. Integrating the first pair of equations in (4.47) yields the similarity variable

$$s \equiv s(x,t) = (x + a)\,(t + q)^{-a_3} = \text{constant},$$

whereas the second pair of DEs in (4.47) determines the similarity solution for (4.34), which reads as

$$F(x,t) = (t+q)^{a_3 - 1}\, \psi(s), \quad \text{where } \psi(s) \text{ is an arbitary function of } s. \tag{4.48}$$

Substituting F, F_x, and F_t into (4.34) results in an ODE for $\psi(s)$

$$\psi'(s) = \frac{p\, \psi(s)}{(p+1)\, \psi(s) - s} \tag{4.49}$$

where $p := (1 - a_3)/a_3$. The solution of (4.49) satisfies the algebraic equation

$$\left[\psi(s)\right]^{-1/p} A + \psi(s) - s = 0, \tag{4.50}$$

where A is a constant of integration. Based on the definitions of s and $\psi(s)$, one derives an algebraic equation for the similarity solution $F(x,t)$ of the form:

$$A\left[F(x,t)\right]^{-1/p} + (t+q)\, F(x,t) - (x+a) = 0, \tag{4.51}$$

The constant A depends on the initial condition $F(x,0) = h(x)$ for (4.34). In particular, when $t = 0$ one obtains the equation satisfied by the initial condition $h(x)$ (for which such similarity solutions F occur)

$$A\,[h(x)]^{-1/p} + q\, h(x) - a = x. \tag{4.52}$$

Based on the definition (4.6) of $h(x)$ as a Laplace transform, we have $h(x) \to 0$ as $x \to \infty$. If we take the limit as $x \to \infty$ in (4.52) we obtain that $p > 0$ or $0 < a_3 < 1$. Since (4.52) holds for all $x \geq 0$, in particular it also holds for $x = 0$. Hence, $A = (a - q\,h(0))\,h(0)^{1/p}$.
Define

$$\mathcal{F}(h) = A\,h^{-1/p} + q\,h - a = x.$$

Differentiating the above with respect to x we obtain

$$\mathcal{F}'(h)\,h'(x) = 1. \tag{4.53}$$

Since $h(x)$ is a completely monotonic function for all $x \geq 0$, we have $h'(x) \leq 0$, so $\mathcal{F}'(h) < 0$ which leads to

$$q - \frac{A}{p}\,[h(x)]^{-\frac{p+1}{p}} < 0. \tag{4.54}$$

Differentiating (4.53) again w.r.t. x and using the complete monotonicity of h we get $\mathcal{F}''(h) > 0$, which gives $A > 0$ and thus $a > q\,h(0)$. Gathering the information obtained so far, we conclude that the PDE (4.34) has a similarity solution $F(x,t)$ given by

$$F(x,t) = (t+q)^{-\frac{p}{p+1}}\,\psi\Big((x+a)\,(t+q)^{-\frac{1}{p+1}}\Big)$$

where $\psi(s)$ satisfies (4.50). In principle, once the function $\psi(s)$ is known, one can use the Laplace transform inversion theorem [23, 117] to obtain the size distribution function $c(\lambda,t)$ in the general form

$$c(\lambda,t) = \frac{(t+q)^{\frac{1-p}{1+p}}\,e^{-\lambda\,(Q(t)+a)}}{\lambda}\,\mathcal{Z}\Big((t+q)^{\frac{1}{p+1}}\,\lambda\Big) \tag{4.55}$$

where $\mathcal{Z}(\mu)$ denotes the inverse Laplace transform of $\psi(s)$.

For some particular values of the constant $p > 0$ one can obtain exact solutions $\psi(s)$ for the algebraic equation (4.50) which lead to the analytic distribution function $c(\lambda,t)$ satisfying (4.2). However, in general the solution of (4.50) cannot be obtained explicitly. To understand the properties of the size distribution function $c(\lambda,t)$, one can investigate the large size ($\lambda \to \infty$) behaviour of $c(\lambda,t)$, for all $t \geq 0$. According to the theory of Laplace transforms (see e.g. [23]) one can deduce the asymptotic behaviour (and properties) of the original function $f(\lambda,t)$ near infinity ($\lambda \to \infty$) when its inverse Laplace transform ($F(x,t)$) is many-valued at the singular point with the largest real part. For this purpose, it is enough to determine the singular points and the asymptotic behaviour of $\psi(s)$ near these points.

For a general first order differential equation

$$v'(s) = \frac{\sigma\, v(s)}{b\, v(s) - m\, s + d} \quad \text{where} \quad \sigma,\, b, m, d \quad \text{are arbitrary constants and} \quad \sigma, m \neq 0$$

one can determine, based on the implicit function theorem, a branch point of the solution $v(s)$ with the largest real part to be given by

$$s_0 = \frac{1}{m} \left(\frac{C_1\, m(m+\sigma)}{\sigma}\, b^{\frac{m}{\sigma}} + d \right)^{\frac{\sigma}{m+\sigma}} \tag{4.56}$$

where C_1 is a constant of integration.

For the function $\psi(s)$ satisfying (4.49) we have $\sigma = p$, $b = p+1$, $m = 1$, $d = 0$ and A defined above. Thus, we obtain that the branch point of $\psi(s)$ is given by

$$s_0 = (p+1)\, \left(A/p\right)^{\frac{p}{p+1}} = (p+1)\, \alpha_0.$$

Using Newton's polygon method (for more details see e.g. [109, 115]), we obtain the asymptotic behaviour of $\psi(s)$

$$\psi(s) \sim \alpha_0 - \sqrt{\frac{2\, \alpha_0\, p}{p+1}}\, \left(s - s_0\right)^{1/2} \quad \text{as} \quad s \to s_0,$$

where $\alpha_0 = s_0/(p+1)$. The dominant small $s \to s_0$ singularity in $\psi(s)$ is a square root branch point which gives an algebraic tail $\sim \lambda^{-3/2}$ in the inverse Laplace transform $\lambda\, c(\lambda, t)$ as $\lambda \to \infty$ (see Theorem 37.2 in [23]). Therefore, the asymptotic behaviour of the inverse Laplace transform of $\psi(s)$ is given by

$$\mathcal{L}^{-1}\{\psi(s)\}(\mu) = \mathcal{Z}(\mu) \sim \frac{1}{2\sqrt{\pi}} \sqrt{\frac{2\, \alpha_0\, p}{p+1}}\; \mu^{-3/2}\, e^{\alpha_0\, (p+1)\, \mu} \quad \text{as} \quad \mu \to \infty$$

which, when substituted into the general formula (4.55) yields the following asymptotic behaviour for the size distribution function $c(\lambda, t)$ for all $t \geq 0$:

$$c(\lambda, t) \sim \frac{1}{\sqrt{2\pi}} \sqrt{\frac{\alpha_0\, p}{p+1}}\, (t+q)^{-\frac{(2p+1)}{2\,(p+1)}}\, \lambda^{-5/2}\, e^{-\left(Q(t)+a-\alpha_0\,(p+1)\,(t+q)^{1/(p+1)}\right)\lambda} \quad \text{as} \quad \lambda \to \infty$$

where $Q(t)$ is obtained from the boundary condition (4.12). Thus $Q(t)$ is given by the following I.V.P.

$$Q'(t) = F(Q(t),\, t) \quad \text{subject to I.C.} \quad Q(0) = 0 \quad \text{where} \quad F(x, t) \text{ satisfies (4.51).}$$

To determine completely the expression of $c(\lambda, t)$, we need to find the function $Q(t)$. This can be obtained by substituting $x = Q(t)$ into (4.51). Thus, we obtain an ODE for $Q(t)$ which later can be used to determine the expression of the first moment of the solution

$$\left[Q'(t)\right]^{-1/p} A + (t+q)\, Q'(t) = Q(t) + a.$$

Differentiating this equation with respect to t gives

$$M_1'(t) \cdot \left\{ t + q - \frac{A}{p} \left[M_1(t)\right]^{-(p+1)/p} \right\} = 0.$$

In this particular case, where no particle source terms are present in the coagulating system, it is expected that the total mass $M_1(t)$ be conserved, i.e. $M_1(t) = M_1(0)$ up to the gel-time T_{gel}. After this moment, $M_1(t)$ starts to decrease. For the expression of the gel-time we use the definition in [96],

$$T_{gel} = -\frac{1}{h'(0^+)} = \frac{A}{p}\left[h(0)\right]^{-\frac{p+1}{p}} - q > 0. \tag{4.57}$$

According to [96], T_{gel} is defined as the instance when the second moment $M_2(t)$ diverges. We detail below the pre and post gelation stages:

In the pre-gelation stage $t \in [0, T_{gel})$, we have $M_1'(t) = 0$, so $Q''(t) = 0$. Also, using the initial condition $Q(0) = 0$ and since $M_1(t) = M_1(0) = h(0)$, we find that $Q(t) = h(0)\, t$, where $h(0)$ satisfies the algebraic equation $A\,[h(0)]^{-1/p} + q\, h(0) = a$ and A, a, $q > 0$ are arbitrary constants.

In the post-gelation regime $t \geq T_{gel}$, the equality $M_1(t) = M_1(0)$ no longer holds, and thus we have $Q''(t) \neq 0$. The latter yields

$$Q'(t) = \left[\frac{p}{A}(t+q)\right]^{-\frac{p}{p+1}}.$$

Integrating the above equation on $[T_{gel}, t]$ and using the continuity of $Q(t)$ (as the primitive of a bounded function) at $t = T_{gel}$, to get $Q(T_{gel}) = h(0)\, T_{gel}$ and the definition of T_{gel}, we obtain

$$Q(t) = -a + (p+1)\left(\frac{A}{p}\right)^{\frac{p}{p+1}} (t+q)^{-\frac{p}{p+1}} = -a + \alpha_0\,(p+1)\,(t+q)^{-\frac{p}{p+1}}, \text{ for } t \geq T_{gel}.$$

Thus we have obtained the following example.

Example 4.1 *(Asymptotic solutions for the pure coagulation equation (4.2))* *Let the initial condition be defined such that* $\lambda\, c(\lambda,0)$ *is the inverse Laplace transform of the function* $h(x)$ *satisfying the algebraic equation*

$$A\,[h(x)]^{-1/p} + q\,h(x) - (x+a) = 0,$$

where A, p, q, $a > 0$ *satisfy conditions which ensure complete monotonicity of* $h(x)$. *Assume the coagulation kernel is* $K(\lambda,\mu) = \lambda\,\mu$ *and the source term is* $g(\lambda,t) = 0$. *Then the solution* $c(\lambda,t)$ *of (4.2) for every* $t \geq 0$ *behaves as follows*

$$c(\lambda,t) \sim \frac{1}{\sqrt{2\pi}}\sqrt{\frac{\alpha_0\,p}{p+1}}\,(t+q)^{-\frac{(2p+1)}{2(p+1)}}\,\lambda^{-5/2}\,e^{-\left(Q(t)+a-\alpha_0\,(p+1)\,(t+q)^{1/(p+1)}\right)\lambda} \quad \textit{as} \quad \lambda \to \infty$$

where

$$Q(t) = \begin{cases} h(0)\,t, & \textit{for} \quad t \in [0, T_{gel}) \\ -a + \alpha_0\,(p+1)\,(t+q)^{-\frac{p}{p+1}}, & \textit{for} \quad t \geq T_{gel} \end{cases}$$

where A, p, q, $a > 0$ *are constants, and* $\alpha_0 = \left(\frac{A}{p}\right)^{\frac{p}{p+1}}$. *Here* T_{gel} *represents the gelation time and is given by* $T_{gel} = \frac{A}{p}\,[h(0)]^{-\frac{p+1}{p}} - q$. *In addition, the total mass* $M_1(t)$ *is given by*

$$M_1(t) = \begin{cases} h(0), & \textit{for} \quad t \in [0, T_{gel}) \\ \alpha_0\,(t+q)^{-\frac{p}{p+1}}, & \textit{for} \quad t \geq T_{gel} \end{cases} \qquad \square$$

Particular choice of constants

In particular, if we choose $p = 1$ and a, $q > 0$ then we obtain the exact solution $\psi(s)$ of the quadratic equation (4.50) as $\psi(s) = \frac{1}{2}\left(s - \sqrt{s^2 - 4A}\right)$. Moreover, we have

$$u(x,t) = F(x+Q(t),t) = \frac{k}{x + Q(t) + a + \sqrt{(x+Q(t)+a)^2 - 2kt - r^2}}$$

where $k := 2A$ and $r^2 := 2qk$. At $t = 0$ we obtain the initial conditions for (4.34) and (4.2), respectively to be

$$h(x) = \frac{k}{x + a + \sqrt{(x+a)^2 - r^2}} \quad \text{and} \quad c_0(\lambda) = \frac{k\,e^{-a\lambda}}{r\,\lambda^2}\,I_1(\lambda\,r),$$

where I_1 represents the modified Bessel function of the first kind [1]. Moreover, in this case, we can calculate the inverse Laplace transform $\mathcal{Z}(\mu)$ of $\psi(s)$ exactly

$$\mathcal{Z}(\mu) = \frac{\sqrt{k}}{\sqrt{2}\,\mu}\,I_1(\mu\sqrt{2\,k})$$

Substituting this result into the general formula (4.55) we obtain an exact family of solutions to the coagulation equation (4.2) and an expression for the total mass for all $t \geq 0$.

Example 4.2 *(**New family of explicit solutions to the pure coagulation equation (4.2)**) Let the initial condition to (4.2) be* $c_0(\lambda) = \frac{k e^{-a\lambda}}{r\lambda^2} I_1(\lambda r)$ *and the source term* $g(\lambda, t) = 0$*. Assume the coagulation kernel* $K(\lambda, \mu) = \lambda \mu$*. Then the solution* $c(\lambda, t)$ *is given by*

$$c(\lambda, t) = \frac{k\, e^{-(Q(t)+a)\,\lambda}}{\lambda^2} \frac{I_1\left(\lambda \sqrt{2\,k\,t + r^2}\right)}{\sqrt{2\,k\,t + r^2}}$$

where $Q(t)$ *is given by*

$$Q(t) = \begin{cases} \frac{k}{a+m}\, t, & \text{for} \quad t \in [0, T_{gel}) \\ \sqrt{2\,k\,t + r^2} - a, & \text{for} \quad t \geq T_{gel} \end{cases}$$

where k, r, $q > 0$, $a \geq r > 0$ *and* $m := \sqrt{a^2 - r^2}$ *are arbitrary constants and the gel-time is given by* $T_{gel} = \frac{m\,r^2}{k\,(a-m)}$*. The expression of the total mass* $M_1(t)$ *is given by*

$$M_1(t) = \begin{cases} \frac{k}{a+m}, & \text{for} \quad t \in [0, T_{gel}) \\ \frac{k}{\sqrt{2\,k\,t+r^2}}, & \text{for} \quad t \geq T_{gel} \end{cases} \qquad \square$$

Remark 4.1 *In particular, if* $a_1 = 0$ *then* $q = 0$*. In this case, we can determine explicitly the initial condition* $h(x)$ *of the Burgers' inviscid equation (4.34) (see Case Ia below).*

Case Ia: Vector field $V = V_4 + a_3\, V_3 + a_2\, V_2$

In this case, the similarity variable and the similarity solutions are given by

$$s \equiv s(x, t) = (x + a)\, t^{-\frac{1}{p+1}} \quad \text{and} \quad F(x, t) = t^{-\frac{p}{p+1}}\, \psi(s)$$

where $a := a_2/a_3$ and $p = (1 - a_3)/a_3$. The function $\psi(s)$ satisfies (4.49) or (4.50), while $F(x, t)$ satisfies the algebraic equation

$$A\left[F(x, t)\right]^{-1/p} + t\, F(x, t) - (x + a) = 0,$$

where A is the constant of integration, which depends on the initial condition $F(x,0) = h(x)$ of (4.34). In particular, when we set $t = 0$ in the equation above we obtain an expression for the initial condition

$$h(x) = \left(\frac{A}{x+a}\right)^p$$

that gives such similarity solutions F as above, where A, p, $a > 0$ arbitrary constants. This explicit expression of $h(x)$ allows us to determine the inverse Laplace transform of $h(x)$, i.e. the initial condition $\lambda\, c_0(\lambda)$ and thus we obtain

$$c_0(\lambda) = \frac{A^p\, \lambda^{p-2}\, e^{-a\,\lambda}}{\Gamma(p)} \quad \text{(the gamma distribution).}$$

Hence, we obtain the asymptotic behaviour of the size distribution $c(\lambda, t)$ of (4.2). Same as in Case I, our results agree with those derived by Ernst et al. in [34] by using the saddle point method (see Eq. (3.13) in [34]). Our result is summarized below:

Example 4.3 *Assume the initial condition* $c_0(\lambda)$ *to (4.2) is given by*

$$c_0(\lambda) = \frac{A^p\, \lambda^{p-2}\, e^{-a\,\lambda}}{\Gamma(p)}$$

where A, p, q, $a > 0$ *are constants. Let the coagulation kernel be* $K(\lambda, \mu) = \lambda\, \mu$ *and the source* $g(\lambda, t) = 0$. *Then the solution* $c(\lambda, t)$ *of (4.2) for every* $t \geq 0$ *behaves as follows*

$$c(\lambda, t) \sim \frac{1}{\sqrt{2\pi}} \sqrt{\frac{\alpha_0\, p}{p+1}}\; t^{-\frac{(2p+1)}{2(p+1)}}\, \lambda^{-5/2}\, e^{-\left(Q(t)+a-\alpha_0\,(p+1)\,t^{1/(p+1)}\right)\lambda} \quad \textit{as} \quad \lambda \to \infty \tag{4.58}$$

where

$$Q(t) = \begin{cases} \beta_0\, t, & \textit{for} \quad t \in [0, T_{gel}) \\ -a + \alpha_0\,(p+1)\, t^{-\frac{p}{p+1}}, & \textit{for} \quad t \geq T_{gel} \end{cases}$$

where $\alpha_0 := \left(\frac{A}{p}\right)^{\frac{p}{p+1}}$, $\beta_0 := \left(\frac{A}{a}\right)^p$ *and* $T_{gel} = \frac{A}{p}\,(\beta_0)^{-\frac{p+1}{p}}$ *is the gel-time. Moreover, the total mass* $M_1(t)$ *is given by*

$$M_1(t) = \begin{cases} \beta_0, & \textit{for} \quad t \in [0, T_{gel}) \\ \alpha_0\, t^{-\frac{p}{p+1}}, & \textit{for} \quad t \geq T_{gel} \end{cases}$$

In particular, if $A = a = p = 1 > 0$ then we obtain the solution in [34].

Remark 4.2 *With the asymptotic large size* ($\lambda \to \infty$) *solutions obtained in Examples 4.1 and 4.3 we recover the asymptotic solution [3.13] in Ernst et al [34]. Here, we have takes* $z_0(t) = Q(t) + a - \alpha_0\,(p+1)\,(t+q)^{1/(p+1)}$, *where* $q > 0$ *and* $q = 0$, *respectively.*

Case Ib: Vector field $V = V_4 + a_2 V_2$

In this case, the generators of the one-parameter group of transformations that leave the PDE (4.34) invariant are given by

$$\xi(x,t) = a_2, \quad \zeta(x,t) = t, \quad \eta(x,t,F) = -F. \tag{4.59}$$

Thus the similarity variable and the similarity solutions become

$$s \equiv s(x,t) = x - \frac{1}{\rho}\ln(t) \quad \text{and} \quad F(x,t) = \psi(s)\,t^{-1},$$

where $\rho := 1/a_2 > 0$. The function $\psi(s)$ satisfies the ODE

$$\psi'(s) = \frac{\rho\,\psi(s)}{\rho\,\psi(s) - 1} \quad \text{with solution} \quad \psi(s) = -\frac{1}{\rho}\,W(-\gamma_0\,\rho\,e^{-s\rho}) \tag{4.60}$$

where we denote by $\gamma_0 = e^{-\rho k} > 0$ (with k a constant of integration) and W is the Lambert W-function defined by the equation $y\exp(y) = x$. Moreover, the function $\psi(s)$ also satisfies the transcendental equation

$$\psi(s) - \frac{1}{\rho}\ln(\psi(s)) = s - \frac{\ln(\gamma_0)}{\rho} \tag{4.61}$$

Using the definition of the function $F(x,t)$ we obtain that F satisfies the equation

$$t\,F(x,t) - \frac{1}{\rho}\ln(F(x,t) = x - \frac{\ln(\gamma_0)}{\rho} \tag{4.62}$$

In particular, when $t = 0$ we obtain the initial conditions for (4.34) and (4.2) for which such similarity solutions F as in (4.62) occur

$$h(x) = \gamma_0\,e^{-\rho x} \quad \text{and} \quad \lambda\,c_0(\lambda) = \gamma_0\,\delta(\lambda - \rho),$$

where the assumption that $\rho > 0$ is made to ensure the complete monotonicity of $h(x)$ for all $x \geq 0$ and the condition $h(x) \to 0$ as $x \to \infty$.

In general, the equation (4.62) cannot be solved explicitly. To understand the behaviour of the solution c to (4.2), we investigate its asymptotic behaviour as $\lambda \to \infty$ for $t \geq 0$. For this purpose, we look at the asymptotic behaviour of its image function $F(x,t)$ near the singular (branch) point with the largest real part.

Since the equation $y\,e^y = x$ has an infinite number of solutions y for each (nonzero) value of x, W has an infinite number of branches. Using the asymptotic formula

$$w(s) = -W(-e^{-s}) \sim 1 - \sqrt{2}\,(s-1)^{1/2}, \quad \text{as } s \to 1$$

we obtain

$$\psi(s) \sim \frac{1}{\rho} - \frac{\sqrt{2\rho}}{\rho}\,(s - s_0)^{1/2} \qquad \text{as} \qquad s \to s_0 := \frac{1 + \ln(\gamma_0\,\rho)}{\rho}.$$

Therefore, the asymptotic behaviour of $F(x,t)$ is given by

$$F(x,t) = \frac{\psi(s)}{t} \sim \frac{1}{\rho\,t} - \frac{\sqrt{2}}{\sqrt{\rho}\,t}\Big(x - x_0(t)\Big)^{1/2} \quad \text{as} \quad x \to x_0(t) := \frac{1 + \ln(\gamma_0\,\rho\,t)}{\rho}$$

where t is fixed. Therefore, the dominant small $x \to x_0(t)$ singularity in $F(x,t)$ is a square root branch point, implying an algebraic tail $\sim \lambda^{-3/2}$ in the inverse Laplace transform $\lambda\,c(\lambda,t)$ as $\lambda \to \infty$ (see Theorem 37.2 in [23]). Thus we obtain the asymptotic behaviour of the original function $c(\lambda,t)$ for all $t \geq 0$ as

$$c(\lambda,t) \sim \frac{1}{t\,\sqrt{2\pi\,\rho}}\,\lambda^{-5/2}\,e^{-\left(Q(t) - \frac{1+\ln(\gamma_0\,\rho\,t)}{\rho}\right)\lambda} \qquad \text{as} \quad \lambda \to \infty,$$

where $Q(t)$ is given by the following I.V.P.

$$Q'(t) = F(Q(t),\,t) \quad \text{subject to I.C.} \quad Q(0) = 0, \quad \text{where} \quad F(x,t) \quad \text{satisfies (4.62).}$$

Substituting $x = Q(t)$ into the equation (4.62) we obtain the following I.V.P. for $Q(t)$

$$t\,Q'(t) - \frac{1}{\rho}\,\ln(Q'(t)) = Q(t) - \frac{\ln(\gamma_0)}{\rho} \quad \text{subject to} \quad Q(0) = 0$$

which by differentiation w.r.t. t yields

$$Q''(t)\cdot\left(t\,Q'(t) - \frac{1}{\rho}\right) = 0.$$

In this case, using again the same definition in [96], we obtain the gel-time: $T_{gel} = \frac{1}{\gamma_0\,\rho}$. Next, we investigate the pre- and post-gelation stages.

In the pre-gelation regime, for $0 \leq t < T_{gel}$ we have $Q''(t) = 0$ with I.C. $Q(0) = 0$, and thus the solution $Q(t) = h(0)\,t = \gamma_0\,t$. On the other hand, in the post-gelation stage, for $t \geq T_{gel}$ we obtain

$$Q'(t) = \frac{1}{\rho\,t} \qquad \text{with I.C.} \quad Q(T_{gel}) = \frac{1}{\rho} \quad \Rightarrow \quad Q(t) = \frac{1 + \ln(\gamma_0\,\rho\,t)}{\rho}.$$

Consequently, we have obtained the following

Example 4.4 *Let γ_0, $\rho > 0$ be arbitrary constants. Suppose the initial condition $c_0(\lambda)$ to (4.2) is $\lambda\, c_0(\lambda) = \gamma_0\, \delta(\lambda - \rho)$, the source $g(\lambda, t) = 0$ and the coagulation kernel $K(\lambda, \mu) = \lambda\, \mu$. Let the function $Q(t)$ be given by:*

$$Q(t) = \begin{cases} \gamma_0\, t, & \text{for} \quad t \in [0, T_{gel}) \\ \frac{1+\ln(\gamma_0\, \rho\, t)}{\rho}, & \text{for} \quad t \geq T_{gel} \end{cases}$$

Then the solution $c(\lambda, t)$ of (4.2) behaves as follows

$$c(\lambda, t) \sim \frac{1}{t\, \sqrt{2\pi\, \rho}}\, \lambda^{-5/2}\, e^{-\left(Q(t) - \frac{1+\ln(\gamma_0\, \rho\, t)}{\rho}\right)\lambda} \qquad \text{as} \qquad \lambda \to \infty \quad \text{and for all} \ \ t \geq 0.$$

The total mass $M_1(t)$ is given by

$$M_1(t) = \begin{cases} \gamma_0, & \text{for} \quad t \in [0, T_{gel}) \\ \frac{1}{\rho\, t}, & \text{for} \quad t \geq T_{gel}. \end{cases}$$

where $T_{gel} = \frac{1}{\gamma_0\, \rho}$, represents the gel-time.

Remark 4.3 *In order to obtain new invariant solutions to the inviscid Burgers' equation (4.34), we have also considered other vector fields in Theorem 4.1. We enumerate a few vector fields for which we have obtained explicit similarity solutions $F(x, t)$:*

(ii) $V_7 + a\, V_1$, *with* $a < 0$ *with the similarity solution* $F(x, t) = \frac{1}{a}\, t - \sqrt{-\frac{2}{a}\left(x - \frac{t^2}{2a}\right)}$

(iii) $V_6 + c\, V_3$, *with* $c \neq 0$, *with the similarity solution* $F(x, t) = \frac{x}{t+c}$

However, none of the similarity solutions we obtained satisfy the definition of Laplace transform, and thus they are of no interest to our study. Other vector fields have been considered, however they lead to Abel's equation of the second kind for which we haven't obtained explicit solutions. For these types of equations, one either uses numerical methods or asymptotic analysis. We have left these vector fields for future work. One can also apply group methods for search of solvable Abel equations (see e.g. [111]).

Summary for Cases I, Ia, Ib in 4.2.2

In Cases I, Ia and Ib, we obtain a more general family of asymptotic solutions that depend on the total mass $M_1(t)$, which also include the solution of Ernst et al. [34] as a particular case (one takes $A = a = p > 0$ and $q = 0$ in Cases I and Ia, or $\rho = \gamma_0 = 1$ in Case Ib). The advantage of our method is that we obtain a general formula for the solution $c(\lambda, t)$ that includes the total mass as part of the solution. In our case we do not need to know the expression of the total mass in advance in order to derive the solution of the coagulation equation as in [34]. The expression of $M_1(t)$ results as a solution to an I.V.P. Furthermore, we provide a more systematic method which does not rely on the saddle point method.

4.2.3 Coagulation kernel $K(\lambda, \mu) = \lambda\,\mu$ and $g(\lambda, t) > 0$ (sources)

In this particular case, the PDE (4.13) reduces to a Burgers' equation with source terms of the form:

$$F_t(x,t) + F(x,t)\,F_x(x,t) = G(x,t) \tag{4.63}$$

Generators for the one-group of transformations

It was proved in 4.2.1 that $\zeta_x(x,t) = 0$ and $\zeta_0(t) = 0$, so $\zeta(x,t) = \zeta_1(t)$ is a function of t only. Thus, (4.25) becomes $2\,\xi_0'(t) = \zeta_1''(t)$, so $\zeta_1'(t) = 2\,\xi_0(t) + a_1$ and $\xi(x,t) = \xi_0(t)\,x + \xi_1(t)$, where a_1 is an arbitrary constant. Moreover, since the generators also satisfy (4.26), we obtain the generators admitted by (4.63) to be

$$\xi(x,t) = \xi_0(t)\,x + \xi_1(t), \quad \zeta(x,t) = \zeta_1(t), \quad \eta(x,t,F) = -[\xi_0(t) + a_1]\,F + \xi_0'(t)\,x + \xi_1'(t)$$

where

$$\begin{aligned} &\zeta_1'(t) = 2\,\xi_0(t) + a_1 \quad \text{and} \\ &[\xi_0(t)\,x + \xi_1(t)]\,G_x + \zeta_1(t)\,G_t + [3\,\xi_0(t) + 2\,a_1]\,G = \xi_0''(t)\,x + \xi_1''(t). \end{aligned} \tag{4.64}$$

In this case, the invariant surface condition (3.11) becomes

$$[\xi_0(t)\,x + \xi_1(t)]\,F_x + \zeta_1(t)\,F_t + [\xi_0(t) + a_1]\,F = \xi_0'(t)\,x + \xi_1'(t).$$

Assume that $\xi_0(t) \neq 0$. The case $\xi_0(t) = 0$ is left for future work. Then, using the definition of $F(x,t)$ as a Laplace transform, it follows that a necessary condition for the above equation to hold for all $x \geq 0$ is $\xi_0'(t) = 0$, so $\xi_0(t) = c_1$ and $\xi_0''(t) =$

0. Thus, the generators for the one-parameter group of Lie point transformations admitted by the equation (4.63) are

$$\xi(x,t) = c_1\,x + \xi_1(t), \quad \zeta(x,t) = \zeta_1(t), \quad \eta(x,t,F) = -(a_1+c_1)\,F + \xi_1'(t).$$

In this case, the invariant surface condition and equation (4.64) take the form

$$[c_1\,x + \xi_1(t)]\,F_x + \zeta_1(t)\,F_t = -(c_1+a_1)\,F + \xi_1'(t) \tag{4.65}$$

$$[c_1\,x + \xi_1(t)]\,G_x + \zeta_1(t)\,G_t = -(3\,c_1+2\,a_1)\,G + \xi_1''(t). \tag{4.66}$$

To solve the equations above, we use the method of characteristics. There are two subcases to consider here. We refer to these cases as Case A and Case B. In both cases we determine the general similarity solutions for the Burgers' equation (4.63) with source terms.

Symmetry reductions for Burgers' equation with sources

Case A. Assume $\zeta_1(t) = 0$, for every $t \geq 0$

Using the definition of $F(x,t)$ as a Laplace transform and letting $x \to \infty$ in (4.65), we obtain $\xi_1'(t) = 0$, so $\xi_1(t) = c_2$ any constant. Thus, the solution of (4.65) becomes

$$F(x,t) = p(t)\,(c_1\,x + c_2)^{-\frac{a_1+c_1}{c_1}} \tag{4.67}$$

where $p(t) > 0$ is an arbitrary function of t and c_1, $c_2 > 0$ and a_1 are arbitrary constants such that $a_1/c_1 > -1$.

Next, we prove that the only condition that guarantees the function $F(x,t)$ vanishes as $x \to \infty$ is that $c_1 = 0$. Indeed, assume the contrary, i.e. $c_1 \neq 0$. To solve the equation (4.65) we use a procedure called "*The Direct Substitution Method*" (see e.g. [13, 14]), that is computationally better than the "*Invariant Form Method*" that we used in Section 4.2.2. Next, we substitute $F(x,t)$ into (4.63) and we obtain that the function $G(x,t)$ is given by the following expression

$$G(x,t) = p'(t)\,(c_1\,x + c_2)^{-\frac{a_1+c_1}{c_1}} - (a_1+c_1)\,p^2(t)\,(c_1\,x + c_2)^{-\frac{2\,a_1+3\,c_1}{c_1}}$$

Substituting $G(x,t)$ above into the determining equation (4.66) we find

$$-p'(t)\,(a_1+c_1)\,(c_1\,x + c_2)^{-\frac{a_1}{c_1}-1} = -p'(t)\,(3\,c_1+2\,a_1)\,(c_1\,x + c_2)^{-\frac{a_1}{c_1}-1}.$$

So, the constants a_1 and c_1 satisfy the relation $a_1 + c_1 = 3\,c_1 + 2\,a_1$, or $a_1 = -2\,c_1$, which fails to satisfy the inequality $a_1/c_1 > -1$ obtained above. Therefore, we have $c_1 = 0$. Thus the generators of the Lie group of point transformations become

$$\xi(x,t) = c_2, \quad \zeta(x,t) = 0, \quad \eta(x,t,F) = -a_1\,F.$$

If $c_2 = 0$ then we have two subcases to consider here:

(a) If $a_1 \neq 0$, then from (4.65) we have the unique solution $F \equiv 0$. This solution yields $G(x,t) = 0$, which contradicts the assumption $G(x,t) > 0$.

(b) If $a_1 = 0$ then there is no nontrivial group of transformations admitted by the Burgers' equation with source terms (4.63).

Therefore, we only consider the case $c_2 \neq 0$ for all $t \geq 0$. Then using $c_1 = 0$, the solution (4.67) becomes

$$F(x,t) = p(t)\,e^{-\frac{a_1}{c_2}x}.$$

Substitution of $F(x,t)$ into the original PDE (4.63) gives rise to a function $G(x,t)$ of the form

$$G(x,t) = p'(t)\,e^{-\frac{a_1}{c_2}x} - \frac{a_1}{c_2}\,p^2(t)\,e^{-\frac{2a_1}{c_2}x}$$

which when substituted into (4.66) gives $a_1\,p'(t)e^{-\frac{a_1}{c_2}x} = 0$, so $p(t) = c_3 > 0$, where c_3 is an arbitrary constant. Thus,

$$F(x,t) = c_3\,e^{-\frac{a_1}{c_2}x} \quad \text{and} \quad G(x,t) = -\frac{a_1}{c_2}\,c_3^2\,e^{-\frac{a_1}{c_2}x}. \tag{4.68}$$

Since $G(x,t) < 0$ then the definition of $G(x,t)$ as a completely monotonic function in x fails to be true. To summarize, there are no completely monotonic functions $G(x,t)$ for which similarity solutions $F(x,t)$ of the form (4.68) exist for the equation (4.63).

Case B. Assume $\zeta_1(t) \neq 0$, for every $t \geq 0$

In this case, the generators of the Lie group of point transformations admitted by the Burgers' equation with source terms (4.63) are given by

$$\xi(x,t) = c_1\,x + \xi_1(t), \quad \zeta(x,t) = \zeta_1(t), \quad \eta(x,t,F) = -(a_1 + c_1)\,F + \xi_1'(t),$$

where $\zeta_1(t) \neq 0$ and $\zeta_1'(t) = 2\,\xi_0(t) + a_1 = 2\,c_1 + a_1$, since $\xi_0(t) = c_1$. So, $\zeta_1(t) = (2\,c_1 + a_1)\,t + c_2$, where c_2 is an arbitrary constant. In addition, using the definition of F_t as a Laplace transform, we can deduce from (4.65) that $\xi_1'(t) = 0$ and thus $\xi_1(t) = c_3$ is an arbitrary constant. We illustrate below a few steps that we take to determine similarity solutions:

Step 1. First, we solve the invariant surface condition (4.65) by using the method of characteristics and obtain that the similarity variable and the similarity solution, respectively are given by

$$s = (x + c_3)|\zeta_1(t)|^{-\frac{c_1}{2c_1+a_1}} \quad \text{and} \quad F(x,t) = (\psi(s) + A_1)\,|\zeta_1(t)|^{-\frac{a_1+c_1}{2c_1+a_1}}$$

where A_1 is an arbitrary constant.

Step 2. Solve the PDE (4.66) for $G(x,t)$ using again the method of characteristics. We obtain

$$G(x,t) = (\varphi(s) + A_2)\,|\zeta_1(t)|^{-\frac{2a_1+3c_1}{2c_1+a_1}} \tag{4.69}$$

where A_2 is an arbitrary constant.

Step 3. Finally, substitute $F(x,t)$ and $G(x,t)$ obtained in Steps 1 and 2 into (4.63) to get

$$\psi(s)\,\psi'(s) - \varphi(s) - \left\{c_1\,s\,\psi'(s) + (a_1 + c_1)\,\psi(s)\right\} + \psi'(s)\,A_1 - (a_1 + c_1)\,A_1 - A_2 = 0,$$

Using the steps above, the generators for the one-group of Lie point transformations become

$$\xi(x,t) = c_1\,x + c_3, \quad \zeta(x,t) = \zeta_1(t) = (2\,c_1 + a_1)\,t + c_2, \quad \eta(x,t,F) = -(c_1 + a_1)\,F$$

where a_1, c_1, c_2, c_3 are arbitrary parameters. Hence, a nontrivial four-parameter Lie group of transformations acting on the (x,t,F)-space is admitted by the Burgers' equation with source terms (4.63).

The infinitesimal generator X associated with the above Lie group of point-transformations can be written as

$$X = a_1\left(t\,\frac{\partial}{\partial t} - F\,\frac{\partial}{\partial F}\right) + c_1\left(x\,\frac{\partial}{\partial x} + 2\,t\,\frac{\partial}{\partial t} - F\,\frac{\partial}{\partial F}\right) + c_2\,\frac{\partial}{\partial t} + c_3\,\frac{\partial}{\partial x}$$

Therefore equation (4.63) admits a Lie algebra $\hat{L}_4$ spanned by the following four vector fields:

$$V_1 = t\,\frac{\partial}{\partial t} - F\,\frac{\partial}{\partial F}, \quad V_2 = x\,\frac{\partial}{\partial x} + 2\,t\,\frac{\partial}{\partial t} - F\,\frac{\partial}{\partial F}, \quad V_3 = \frac{\partial}{\partial t}, \quad V_4 = \frac{\partial}{\partial x}$$

The commutator table for the Lie algebra arising from these infinitesimal generators is given in Table 4.2.

$[V_i, V_j]$	V_1	V_2	V_3	V_4
V_1	0	0	$-V_3$	0
V_2	0	0	$-2\,V_3$	$-V_4$
V_3	V_3	$2\,V_3$	0	0
V_4	0	V_4	0	0

Table 4.2: Commutator $[V_i, V_j]$ table for the Lie algebra $\hat{L}_4$ spanned by V_i and V_j.

We consider first the case of the most general one-parameter group of symmetry transformations by choosing a general linear combination $v = a_1\,V_1 + c_1\,V_2 + c_2\,V_3 + c_3\,V_4$, where c_1, $c_2 \neq 0$, c_3 are arbitrary and $2\,c_1 + a_1 \neq 0$. Using the method of characteristics to solve the invariant surface condition (4.45), we obtain the following general result:

Theorem 4.2 *Let A_1, A_2 be arbitrary constants. In addition, assume c_1, $c_2 \neq 0$, c_3 arbitrary and $2\,c_1 + a_1 \neq 0$. Let $\varphi(s) \to 0$, as $s \to \infty$. In addition assume $\varphi(s) + A_2 > 0$ for all s, and $-\varphi'(s)$ is a completely monotonic function for all $s \in \mathbb{R}$, where*

$$s = (x + c_3)|\zeta_1(t)|^{-\frac{c_1}{2\,c_1 + a_1}}$$

represents the similarity variable, where $\zeta_1(t) = (2\,c_1 + a_1)\,t + c_2$. Assume the function $G(x,t)$ has the similarity form given by

$$G(x,t) = (\varphi(s) + A_2)\,|\zeta_1(t)|^{-\frac{2\,a_1 + 3\,c_1}{2\,c_1 + a_1}}$$

Then the partial differential equation (4.63) has a similarity solution given by

$$F(x,t) = (\psi(s) + A_1)\,|\zeta_1(t)|^{-\frac{a_1 + c_1}{2\,c_1 + a_1}}$$

where $\psi(s)$ satisfies the ODE

$$\psi'(s) = \frac{\varphi(s) + (a_1 + c_1)\,\psi(s) + A_2 + (a_1 + c_1)\,A_1}{\psi(s) + A_1 - c_1\,s} \tag{4.70}$$

The constants a_1 and c_1 are such that:

(a) $\psi(s)$ *vanishes to zero as* $s \to \infty$;

(b) $\psi(s)$ *satisfies* $\psi(s) + A_1 > 0$;

(c) $-\psi'(s)$ *is a completely monotonic function for all* s.

Remark 4.4 *Without loss of generality we may assume the constants* A_1 *and* A_2 *in Theorem 4.2 to be zero. In addition, we also consider the constant* $c_3 \neq 0$ *as otherwise we obtain solutions that are not realistic, from a physical point of view. Future work will investigate a few examples of constants* a_1 *and* c_1 *for which the function* ψ *to (4.70) satisfies conditions (a-c) in Theorem 4.2. To illustrate a few examples of similarity solutions we consider below a few one-parameter subalgebras generated by* X *above.*

Case I: Vector field $V = a_1 V_1 + c_1 V_2 + c_2 V_3 + c_3 V_4$

Our aim is to look for examples of functions $\varphi(s)$ that are completely monotonic in s and for which the ODE (4.70) can be solved explicitly. By solving (4.70) we obtain $\psi(s)$. Since we are interested only in those functions $\psi(s)$ that are completely monotonic in s, we need to impose certain conditions (restrictions) on the non-zero constants a_1 and c_1 satisfying $2a_1 + c_1 \neq 0$. By doing so, we obtain similarity solutions $F(x,t)$ for the PDE (4.63), which in some cases become exact solutions. We present an example of such an exact solution to (4.2) below.

Example 4.5 *(i)* *Assume* $a, k, q > 0$ *are arbitrary constants such that* $a > kq$. *Let the coagulation kernel be* $K(\lambda, \mu) = \lambda\mu$. *If the source term* $g(\lambda, t)$ *is given by*

$$g(\lambda, t) = \frac{k\, e^{-\lambda(Q(t)+a)}}{(t+q)\,\lambda^2}\, I_1(k\lambda t + k\lambda q),$$

where I_1 *is the modified Bessel function of the first kind [1], then the solution to the coagulation equation (4.2) is given by*

$$c(\lambda, t) = \frac{k\, e^{-\lambda(Q(t)+a)}}{\lambda^2}\, I_1(k\lambda t + k\lambda q),$$

where the function $Q(t)$ *is given by*

$$Q(t) = \begin{cases} \frac{t\,k^2\,(t+2\,q)}{2\,(a+\sqrt{a^2-k^2\,q^2})} & \text{for } \; 0 \le t < T_{gel} \\ k\,(t+q) - a & \text{for } \; t \ge T_{gel} \end{cases} \tag{4.71}$$

T_{gel} *represents the gelation time given by*

$$T_{gel} = \frac{a - kq + \sqrt{a^2 - k^2\,q^2}}{k} \tag{4.72}$$

Let the initial condition of (4.2) be $c_0(\lambda) = k\,e^{-a\,\lambda}\,\frac{I_1(k\,q\,\lambda)}{\lambda^2}$. *In addition, the total mass* $M_1(t)$ *is given by*

$$M_1(t) = \begin{cases} \frac{k^2\,(t+q)}{a+\sqrt{a^2-k^2\,q^2}} & \text{for } \; 0 \le t < T_{gel} \\ k & \text{for } \; t \ge T_{gel} \end{cases} \tag{4.73}$$

(ii) *Assume* $a, k, q > 0$ *are arbitrary constants such that* $a = k\,q$. *Then gelation occurs instantaneously, i.e.* $T_{gel} \equiv 0$.

Proof. Indeed, consider the particular example $\varphi(s) = \psi(s)$. In this case $\psi(s)$ satisfies the ODE:

$$\psi'(s) = \frac{p\,\psi(s)}{\psi(s) - c_1\,s} \quad \text{where} \quad p = a_1 + c_1 + 1, \tag{4.74}$$

or $\psi(s)$ satisfies the algebraic equation

$$A\left[\psi(s)\right]^{-\frac{c_1}{p}} + \frac{1}{c_1 + p}\,\psi(s) - s = 0,$$

where A is a constant of integration and c_1 and p satisfy the condition $c_1/p > 0$ in order to ensure complete monotonicity for the function $\psi(s)$. One can use a similar analysis as for $\psi(s)$ in (4.51) and obtain the asymptotic behaviour of $\psi(s)$ near the branch point s_0 of $\psi(s)$.

In particular, we choose the constants $p = c_1 = 1$. Moreover, if we denote by $k := \sqrt{2\,A}$, $a := c_3$ and $q := c_2$ and assume $a,\ q > 0$, then, $a_1 = -1$ and in this case the similarity solution $F(x,t)$ and the function $G(x,t)$ become

$$F(x,t) = \frac{x+a}{t+q} - \sqrt{\left(\frac{x+a}{t+q}\right)^2 - k^2} \text{ and } G(x,t) = \frac{1}{t+q}\left\{\frac{x+a}{t+q} - \sqrt{\left(\frac{x+a}{t+q}\right)^2 - k^2}\right\}$$

Therefore, the initial condition $F(x,0) = h(x)$ becomes

$$h(x) = \frac{x+a}{q} - \sqrt{\left(\frac{x+a}{q}\right)^2 - k^2}$$

Next, let us prove that (4.73) and (4.72) hold. Indeed, using the boundary condition (4.12) it follows that $Q(t)$ satisfies the I.V.P.

$$Q'(t) = \frac{Q(t)+a}{t+q} - \sqrt{\left(\frac{Q(t)+a}{t+q}\right)^2 - k^2} \quad \text{subject to I.C.} \quad Q(0) = 0. \tag{4.75}$$

If we denote by $v(t) := \frac{Q(t)+a}{t+q}$ then (4.75) simplifies to an I.V.P. for $v(t)$

$$\frac{dv}{\sqrt{v^2-k^2}} = -\frac{dt}{t+q} \quad \text{subject to I.C.} \quad v(0) = \frac{a}{q}.$$

Thus $v(t)$ satisfies

$$\sqrt{v^2(t)-k^2} = \frac{a+\sqrt{a^2-k^2\,q^2}}{t+q} - v(t) \tag{4.76}$$

The solution of (4.76) is given by

$$v(t) = \frac{a+\sqrt{a^2-k^2\,q^2}}{2\,(t+q)} + \frac{k^2\,(t+q)}{2\,(a+\sqrt{a^2-k^2\,q^2})}. \tag{4.77}$$

The expression of $v(t)$ obtained in (4.77) is valid only for values of $t \in [0, T_c)$ where T_c corresponds to the time t such that the following inequalities hold

$$k \leq v(t) \leq \frac{a+\sqrt{a^2-k^2\,q^2}}{t+q}$$

Thus, we obtain

$$T_c = \frac{a - kq + \sqrt{a^2-k^2\,q^2}}{k}$$

On the other hand, using the definition of the gelation time [70, 96] as the instance when the second moment of solution $M_2(t)$ diverges and the definition $M_2(t) = -F_x(Q(t), t)$, we obtain that T_{gel} is given by

$$T_{gel} = \inf\{t \geq 0 \quad \text{s.t.} \quad v(t) = k\} = T_c$$

Hence, the expression (4.77) holds for $t \in [0, T_{gel})$. In addition, the expression in (4.77) yields the formula for the function $Q(t)$ obtained in (4.71) and the expression for the total mass, $M_1(t)$ in the pre-gelation regime, as

$$M_1(t) = \frac{k^2\,(t+q)}{2\,(a+\sqrt{a^2-k^2\,q^2})}, \qquad \forall t \in [0, T_{gel})$$

In the post-gelation regime, we use as an initial condition the expression of $v(t)$ in (4.77) at $t = T_{gel}$ to ensure continuity of $Q(t)$ and thus of $M_1(t)$ at the gel-time. We obtain $v(T_{gel}) = k$. Moreover, for any $t \geq T_{gel}$ we have $v(t) = k$ and the solution of (4.75) becomes

$$Q(t) = k\,(t+q) - a, \qquad \forall t \geq T_{gel} \tag{4.78}$$

This expression yields the formula in (4.73) and thus the total mass is constant for $t \geq T_{gel}$, which completes the proof. □

Case II: Vector field $V = c_1\, V_2 + c_2\, V_3 + c_3\, V_4$

In this case, the generators of the one-group of Lie point transformations admitted by the Burgers' equation with sources (4.63) become

$$\xi(x,t) = c_1\, x + c_3, \quad \zeta(x,t) = 2\, c_1\, t + c_2, \quad \eta(x,t,F) = -c_1\, F,$$

where $c_1 \neq 0$. The case $c_1 = 0$ is treated separately as Case III. Then the following result holds

Example 4.6 ***(Similarity solutions for the Burgers' equation with sources (4.63))*** *Let p, $q > 0$ and $m < -1$ be arbitrary constants such that*

$$\left|\ln\left(-\frac{2}{A^2\,(1+m)}\right)\right| > (1-m)\,\sqrt{q} \quad \textit{where} \quad A = \frac{\exp\left(\frac{(1-m)}{2}\,\sqrt{q}\right)}{p\left(\frac{a}{\sqrt{q}}\right)^{\frac{1-m}{2}} + \sqrt{p^2\left(\frac{a}{\sqrt{q}}\right)^{1-m} + \frac{2}{1+m}}}.$$

Assume the initial condition of (4.63) is given by

$$h(x) = \frac{p}{q}\left(x + a - \sqrt{(x+a)^2 + \frac{2\,q^{-\frac{(m-1)}{2}}}{p^2\,(1+m)}\,(x+a)^{1+m}}\right)$$

The function $h(x)$ is well-defined and completely monotonic for values of x such that

$$x \geq \left(-\frac{2}{p^2\,(1+m)}\,q^{-\frac{(m-1)}{2}}\right)^{\frac{1}{1-m}} - a,$$

where $a > 0$ is arbitrary. In addition, for $x > \frac{c_3}{c_2}\,t$, assume the function $G(x,t)$ is given by

$$G(x,t) = (x+a)^m\,(2\,p\,t + q)^{-\frac{3+m}{2}}.$$

Then the similarity solution $F(x,t)$ to (4.63) has the form

$$F(x,t) = \frac{p}{2\,p\,t+q}\left\{x+a-\sqrt{(x+a)^2+\frac{2\,(2\,p\,t+q)^{-\frac{m-1}{2}}}{p^2\,(1+m)}\,(x+a)^{1+m}}\right\}$$

where

$$Q(t) = \begin{cases} \sqrt{2pt+q}\left(\frac{A^2\exp\left(-(1-m)\sqrt{2pt+q}\right)-\frac{2}{1+m}}{2\,A\,p\,\exp\left(-\frac{(1-m)}{2}\sqrt{2pt+q}\right)}\right)^{\frac{2}{1-m}} - a, & \textit{for} \quad 0 \le t < T_{gel} \\ \sqrt{2pt+q}\left(-\frac{2}{p^2\,(1+m)}\right)^{\frac{1}{1-m}} - a, & \textit{for} \quad t \ge T_{gel} \end{cases}$$

where

$$T_{gel} = \frac{1}{2\,p(1-m)^2}\left[\ln\left(-\frac{2}{A^2\,(1+m)}\right)\right]^2 - \frac{q}{2p} > 0.$$

Proof. Indeed, according to Theorem 4.2, the similarity solution and the function $G(x,t)$ take the form

$$F(x,t) = \frac{\psi(s)}{|\zeta_1(t)|^{1/2}} \quad \text{and} \quad G(x,t) = \frac{\varphi(s)}{|\zeta_1(t)|^{3/2}} \quad \text{where} \quad s = (x+c_3)\,|\zeta_1(t)|^{-1/2}$$

is the similarity variable and $\zeta_1(t) = 2\,c_1\,t + c_2$. Moreover, (4.70) becomes

$$\psi'(s) = \frac{\varphi(s) + c_1\,\psi(s)}{\psi(s) - c_1\,s} \tag{4.79}$$

Since (4.79) is an exact ODE, its solution can be determined by solving the algebraic equation

$$\frac{\psi^2(s)}{2} - c_1\,s\,\psi(s) - \int^s \varphi(s)\,ds + A = 0 \quad \Rightarrow$$

$$\psi(s) = c_1\,s \pm \sqrt{(c_1\,s)^2 - 2\left(A - \int^s \varphi(s)\,ds\right)}$$

where $\varphi(s)$ is a completely monotonic function in s such that $c_1^2\,s^2 + 2\int^s \varphi(s)\,ds - 2\,A > 0$. The variety of functions $\varphi(s)$ that are completely monotonic in s such that $\psi(s)$ itself is completely monotonic and also vanishes to zero as $s \to \infty$ is limited. We have investigated a few such examples of functions $\varphi(s)$. However, we illustrate below one particular interesting example for which we obtain the expression of the total mass of the solution explicitly for all $t \ge 0$ and also the gel-time T_{gel}.

First, we denote by $a := c_3$ and assume $\varphi(s) = s^m$, where $m < 0$ to ensure the definitions of F and G are both satisfied. Then we obtain

$$\psi(s) = c_1\, s - \sqrt{c_1^2\, s^2 + \frac{2\,A}{1+m} + \frac{2\,s^{1+m}}{1+m}} \tag{4.80}$$

Therefore the similarity solution becomes

$$F(x,t) = |\zeta_1(t)|^{-1} \left\{ c_1\,(x+a) - \sqrt{c_1^2\,(x+a)^2 + \frac{2\,A}{1+m}\,|\zeta_1(t)| + \frac{2\,|\zeta_1(t)|^{-\frac{1+m}{2}}}{1+m}\,(x+a)^{1+m}} \right\}$$

and $G(x,t) = (x+a)^m\, |\zeta_1(t)|^{-\frac{m+3}{2}}$, where $\zeta_1(t) = 2\,p\,t + c_2$.

In order to obtain an explicit formula for the total mass, we set $A = 0$, and denote by $p := c_1$. In addition, we assume $m < -1$, such that $F(x,t)$ vanishes to zero as $x \to \infty$ and also $p > 0$ to keep the complete monotonicity of $F(x,t)$. With these notations and assumptions we obtain that $G(x,t)$ and $F(x,t)$ are given by

$$G(x,t) = (x+a)^m\, |2\,p\,t + c_2|^{-\frac{m+3}{2}},$$

and

$$F(x,t) = \frac{p}{|2\,p\,t + c_2|} \left\{ x + a - \sqrt{(x+a)^2 + \frac{2\,|2\,p\,t + c_2|^{-\frac{m-1}{2}}}{p^2\,(1+m)}\,(x+a)^{1+m}} \right\} \tag{4.81}$$

When $t = 0$, if we denote by $q := |c_2| > 0$ then we obtain the initial condition $F(x,0) = h(x)$ of (4.63) to be

$$h(x) = \frac{p}{q} \left(x + a - \sqrt{(x+a)^2 + \frac{2\,q^{-\frac{(m-1)}{2}}}{p^2\,(1+m)}\,(x+a)^{1+m}} \right)$$

Notice that $h(x)$ is well-defined for values of x such that

$$x \geq -a + (-\gamma)^{\frac{1}{1-m}} \quad \text{where} \quad \gamma := \frac{2\,q^{-\frac{m-1}{2}}}{p^2\,(1+m)} < 0. \tag{4.82}$$

For these values of x it can be shown that $h(x)$ is completely monotonic. Indeed, we have

$$h(x) = \frac{p}{q} \left(x + a - \sqrt{(x+a)^2 + \gamma\,(x+a)^{1+m}} \right) \geq 0$$

One can calculate the derivative $h'(x)$ and obtain that $h'(x)$ is a product of two completely monotonic functions $g_1(x)$ and $g_2(x)$ defined by

$$g_1(x) = \frac{p^2}{q^2} \left[(x+a)^m + \frac{q}{p\,\gamma\,(1+m)}\,h(x) \right] \quad \text{and} \quad g_2(x) = -\left[\frac{p}{q}\,(x+a) - h(x) \right]^{-1}$$

for all values of x satisfying (4.82). It is not straightforward to obtain the inverse Laplace transform of the function $h(x)$, and thus an exact formula for $c_0(\lambda)$. Moreover, obtaining exact solutions to (4.2) may not be possible. For this purpose, we restrict our attention to finding an explicit formula for $Q(t)$ and thus the total mass for all $t \geq 0$ and the expression for the gel-time. For simplicity we assume $c_2 > 0$. We start with the derivation of $Q(t)$.

Using the condition (4.12), i.e. $Q'(t) = F(Q(t), t)$ we obtain

$$Q'(t) = \frac{p}{\sqrt{2pt+q}} \left\{ \frac{Q(t)+a}{\sqrt{2pt+q}} - \sqrt{\left(\frac{Q(t)+a}{\sqrt{2pt+q}}\right)^2 + \frac{2}{p^2(1+m)} \left(\frac{Q(t)+a}{\sqrt{2pt+q}}\right)^{1+m}} \right\} \tag{4.83}$$

subject to I.C. $Q(0) = 0$. To simplify (4.83), we denote by $v(t) := \frac{Q(t)+a}{\sqrt{2pt+q}}$. Then (4.83) becomes a separable ODE

$$\frac{dv}{\sqrt{p^2 v^2 + \frac{2v^{1+m}}{1+m}}} = -\frac{dt}{\sqrt{2pt+q}} \quad \text{subject to} \quad v(0) = \frac{a}{\sqrt{q}}$$

The above is equivalent to

$$\frac{v^{-\frac{m+1}{2}}}{\sqrt{\left(p v^{\frac{1-m}{2}}\right)^2 - \left(\sqrt{-\frac{2}{1+m}}\right)^2}} \, dv = -\frac{dt}{\sqrt{2pt+q}}$$

Using the substitution $z = p v^{\frac{1-m}{2}}$ we obtain

$$z(t) + \sqrt{z^2(t) + \frac{2}{1+m}} = A \exp\left(-\frac{(1-m)}{2}\sqrt{2pt+q}\right) \tag{4.84}$$

where

$$A = \frac{\exp\left(\frac{1-m}{2}\sqrt{q}\right)}{p\left(\frac{a}{\sqrt{q}}\right)^{\frac{1-m}{2}} + \sqrt{p^2\left(\frac{a}{\sqrt{q}}\right)^{1-m} + \frac{2}{1+m}}}$$

where $z(t) = p\,[v(t)]^{\frac{1-m}{2}}$ and the constants a, p, q, m satisfy $p^2\left(\frac{a}{\sqrt{q}}\right)^{1-m} > -\frac{2}{1+m}$. Solving (4.84) we obtain

$$v(t) = \left[\frac{A^2 \exp\left((m-1)\sqrt{2pt+q}\right) - \frac{2}{1+m}}{2Ap\exp\left(-\frac{(1-m)}{2}\sqrt{2pt+q}\right)}\right]^{\frac{2}{1-m}} \tag{4.85}$$

However, the expression for $v(t)$ obtained in (4.85) is valid only for values of $t \in [0, T_c)$, where T_c is defined as an upper bound of the solution to the system of inequalities

$$z(t) \geq -\Big(-\frac{2}{1+m}\Big)^{1/2} \quad \text{and} \quad z(t) \leq A \exp\Big(-\frac{(1-m)}{2}\sqrt{2pt+q}\Big).$$

We obtain that T_c is given by

$$T_c = \frac{1}{2p(1-m)^2}\Big[\ln\Big(-\frac{2}{A^2(1+m)}\Big)\Big]^2 - \frac{q}{2p}.$$

Using the definition of the gel-time as in the previous case or [34, 70] we find that $M_2(t) = -F_x(Q(t), t)$ diverges at t such that $z^2(t) = -2/(1+m)$, which gives us $T_{gel} = T_c$. The gel-time T_{gel} is greater than zero provided that $\ln\Big(-\frac{2}{A^2(1+m)}\Big) > \sqrt{q}\,(1-m)$ holds. Therefore, the expression of $v(t)$ given in (4.85) is valid up to the gelation time. As a result, the function $Q(t)$ can also be obtained

$$Q(t) = \sqrt{2pt+q}\left(\frac{A^2\exp\Big(-(1-m)\sqrt{2pt+q}\Big) - \frac{2}{1+m}}{2Ap\exp\Big(-\frac{(1-m)}{2}\sqrt{2pt+q}\Big)}\right)^{\frac{2}{1-m}} - a, \quad \text{for} \quad 0 \leq t < T_{gel}$$

The total mass is given by $M_1(t) = Q'(t)$, so

$$M_1(t) = \left\{\frac{A}{2p}\exp\Big(-\frac{(1-m)}{2}\sqrt{2pt+q}\Big) - \frac{1}{Ap(1+m)}\exp\Big(\frac{(1-m)}{2}\sqrt{2pt+q}\Big)\right\}^{\frac{1+m}{1-m}}$$
$$\left\{\frac{A}{2}\exp\Big(-\frac{(1-m)\sqrt{2pt+q}}{2}\Big)\big[(2pt+q)^{-1/2} - 1\big] - \right.$$
$$\left.\frac{1}{A(1+m)}\exp\Big(\frac{(1-m)\sqrt{2pt+q}}{2}\Big)\big[(2pt+q)^{-1/2} + 1\big]\right\}$$

On the other hand, in the post-gelation regime, we have that

$$v(t) = \Big[-\frac{2}{(1+m)p^2}\Big]^{\frac{1}{a-m}} \quad \text{for} \quad t \geq T_{gel}.$$

This yields an expression for $Q(t)$ and $M_1(t)$ of the form

$$Q(t) = \sqrt{2pt+q}\Big[-\frac{2}{(1+m)p^2}\Big]^{\frac{1}{1-m}} - a \quad \text{and} \quad M_1(t) = \Big[-\frac{2}{(1+m)p^2}\Big]^{\frac{1}{1-m}}\frac{p}{\sqrt{2pt+q}}$$

where both formulas hold for $t \geq T_{gel}$. $\square$

Remark 4.5 *Obtaining an explicit expression for* $c(\lambda, t)$ *requires the calculation of the inverse Laplace transform of* $F(x,t)$ *in (4.81), since* $c(\lambda,t) = \frac{e^{-\lambda Q(t)}}{\lambda}\,\mathcal{L}^{-1}\{F(x,t)\}(\lambda,t)$, *where* $\mathcal{L}^{-1}$ *denotes the inverse Laplace transform of* $F(x,t)$. *We provide below a formal series solution* c *for the coagulation equation.*

Example 4.7 ***(Formal series solution for the coagulation equation (4.2))*** *Assume the coagulation kernel is* $K(\lambda,\mu) = \lambda\,\mu$. *Assume the source term is given by*

$$g(\lambda,t) = \frac{\lambda^{-m-2}\,(2\,p\,t+q)^{-\frac{3+m}{2}}}{\Gamma(-m)}\,e^{-\lambda\,(Q(t)+a)},$$

where $Q(t)$ *is defined in Example 4.6. Then the solution* $c(\lambda,t)$ *of (4.2) is given by the following formal series*

$$c(\lambda,t) = \frac{p\,e^{-(Q(t)+a)\,\lambda}}{\lambda^2\,(2pt+q)}\sum_{k=1}^{\infty}\frac{(2k-2)!}{2^{2k-1}k!(k-1)!}\left(\frac{2\,(2pt+q)^{\frac{1-m}{2}}}{p^2\,(-1-m)}\right)^k\frac{1}{\Gamma((1-m)k-1)}\,\lambda^{(1-m)\,k}.$$

Proof. Formally expanding the square root and taking the inverse Laplace transform term by term we obtain

$$\begin{aligned}
\mathcal{L}^{-1}\{F(x,t)\}(\lambda,t) &= \frac{p}{2pt+q}\,\mathcal{L}^{-1}\left\{x+a-(x+a)\sqrt{1+\frac{2\,(2pt+q)^{\frac{1-m}{2}}}{p^2\,(1+m)}\,(x+a)^{m-1}}\right\}(\lambda,t)\\
&= \frac{-p}{2pt+q}\sum_{k=1}^{\infty}\left(\frac{2\,(2pt+q)^{\frac{1-m}{2}}}{p^2\,(1+m)}\right)^k\binom{1/2}{k}\,\mathcal{L}^{-1}\left\{\frac{1}{(x+a)^{(1-m)\,k}}\right\}(\lambda,t)\\
&= \frac{p\,e^{-a\lambda}}{(2pt+q)\,\lambda^2}\sum_{k=1}^{\infty}a_k(t)\,\lambda^{(1-m)\,k}
\end{aligned}$$

where $\binom{\sigma}{k}$ is the binomial coefficient, defined by $\binom{\sigma}{k} = \frac{\sigma(\sigma-1)(\sigma-2)\ldots(\sigma-k+1)}{k!}$ and where the coefficients are

$$\begin{aligned}
a_k(t) &= \binom{1/2}{k}\left(\frac{2\,(2pt+q)^{\frac{1-m}{2}}}{p^2\,(1+m)}\right)^k\frac{-1}{\Gamma((1-m)k-1)} > 0 &\quad (4.86)\\
&= \frac{(2k-2)!}{2^{2k-1}k!(k-1)!}\left(\frac{2\,(2pt+q)^{\frac{1-m}{2}}}{p^2\,(-1-m)}\right)^k\frac{1}{\Gamma((1-m)k-1)} &\quad (4.87)
\end{aligned}$$

Since $m < -1$ then the series $\sum_{k=1}^{\infty} a_k(t)\, \lambda^{(1-m)\,k}$ with positive terms is convergent for all values of $\lambda \geq 0$. Therefore, the solution $c(\lambda, t)$ to the coagulation equation (4.2) is given by the following convergent series with positive terms (for all $\lambda \geq 0$):

$$c(\lambda, t) = \frac{p\, e^{-(Q(t)+a)\,\lambda}}{\lambda^2\,(2pt+q)} \sum_{k=1}^{\infty} \frac{(2k-2)!}{2^{2k-1}k!(k-1)!} \left(\frac{2\,(2pt+q)^{\frac{1-m}{2}}}{p^2\,(-1-m)} \right)^k \frac{1}{\Gamma((1-m)k-1)}\, \lambda^{(1-m)\,k}$$

where $Q(t)$ is defined in Example 4.6. In particular, when $t = 0$ we obtain the initial condition of (4.2) to be given by the convergent series with positive terms

$$c_0(\lambda) = \frac{p\, e^{-a\,\lambda}}{q\,\lambda^2} \sum_{k=1}^{\infty} \frac{(2k-2)!}{2^{2k-1}k!(k-1)!} \left(\frac{2\,q^{\frac{1-m}{2}}}{p^2\,(-1-m)} \right)^k \frac{1}{\Gamma((1-m)\,k-1)}\, \lambda^{(1-m)\,k} \qquad \square$$

Case III: Vector field $V = c_2\, V_3 + c_3\, V_4$

Consider the infinitesimal generator of the point symmetry group of the form $V = c_2\, V_3 + c_3\, V_4$, where $c_2,\ c_3 \neq 0$. In this case, the generators for the one-group of Lie point transformations admitted by the Burgers equation with sources (4.63) become

$$\xi(x,t) = c_3, \quad \zeta(x,t) = c_2, \quad \eta(x,t,F) = 0.$$

Using the method of characteristics to solve the invariant surface condition (4.45), we obtain the following result:

Theorem 4.3 *Let $c_2, c_3 \neq 0$ be some arbitrary constants. Let $\varphi(s) \to 0$, as $s \to \infty$ and $\varphi(s)$ is a completely monotonic function in s, where $s = x - \frac{c_3}{c_2}\, t$, represents the similarity variable. Assume the function $G(x,t)$ has the similarity form $G(x,t) = \varphi(s)$. Then the partial differential equation (4.63) has a similarity solution given by*

$$F(x,t) = \psi(s) + \frac{c_3}{c_2} \tag{4.88}$$

where $\psi(s)$ satisfies the ODE

$$\psi'(s) = \frac{\varphi(s)}{\psi(s)}. \tag{4.89}$$

The constants c_2 and c_3 are chosen such that the function $\psi(s) \to 0$ as $s \to \infty$. In addition, $\psi(s)$ satisfies $\psi(s) + \frac{c_3}{c_2} > 0$ and $-\psi'(s)$ is a completely monotonic function for all s.

Equivalently, $\psi(s)$ satisfies the equation

$$\frac{\psi^2(s)}{2} = \int^s \varphi(s)\,ds + A_2 \quad or \quad \psi(s) = \pm\sqrt{2}\Big(\int^s \varphi(s)\,ds + A_2\Big)^{1/2} \tag{4.90}$$

where $\varphi(s)$ is a completely monotonic function in s such that $A_2 + \int^s \varphi(s)\,ds \geq 0$ and A_2 is an arbitrary constant.

Remark 4.6 *The complete monotonicity of the function $\psi(s) + \frac{c_3}{c_2}$ and (4.89) imply that $\psi(s) \leq 0$, for all $s \in \mathbb{R}$.*

One particular example that provides a family of similarity solutions $F(x,t)$ to (4.63) is

Example 4.8 *Let $w(s)$ be a function that satisfies the following conditions:*

(H1) $w(s) > 0$, *for every* $s > 0$;

(H2) $w'(s)$ *is completely monotonic in* s;

(H3) $\lim_{s\to\infty} w'(s)\,e^{-w(s)} = 0$ *and* $\lim_{s\to\infty} w(s) = \infty$.

Assume the initial condition of (4.63) is given by

$$h(x) = \frac{c_3}{c_2}\left(1 - \sqrt{1 - \frac{2\,c_2^2}{c_3^2}\,e^{-w(x)}}\right) \tag{4.91}$$

In addition, assume

$$G(x,t) = w'\Big(x - \frac{c_3}{c_2}\,t\Big)\,e^{-w(x - \frac{c_3}{c_2}\,t)} \tag{4.92}$$

where c_2 and c_3 are arbitrary constants such that $\frac{c_3}{c_2} \geq \sqrt{2}$.
Then the Burgers' equation with sources (4.63) admits a family of similarity solutions of the form

$$F(x,t) = \frac{c_3}{c_2}\left(1 - \sqrt{1 - \frac{2\,c_2^2}{c_3^2}\,e^{-w(x - \frac{c_3}{c_2}\,t)}}\right) \tag{4.93}$$

Proof. Indeed, consider the function $\varphi(s) = w'(s)\,e^{-w(s)}$. Then the solution to (4.90) is

$$\psi(s) = \pm\sqrt{2}\,\sqrt{A_2 - e^{-w(s)}}.$$

Moreover, from (4.88) we obtain

$$F(x,t) = \frac{c_3}{c_2} - \sqrt{2\,A_2 - 2\,e^{-w(s)}}.$$

Since $w(s) \to \infty$ as $s \to \infty$ then in order to ensure that $F(x,t) \to 0$ as $x \to \infty$ for all $t \geq 0$ we choose $\frac{c_3}{c_2}$, $A_2 > 0$ such that $2\,A_2 = \frac{c_3^2}{c_2^2}$. With this choice of constants, we obtain

$$F(x,t) = \sqrt{2\,A_2}\left\{1 - \sqrt{1 - \frac{1}{A_2}\,e^{-w\left(x-\frac{c_3}{c_2}t\right)}}\right\}$$

Moreover, the function $G(x,t)$ is given by $G(x,t) = w'\left(x - \frac{c_3}{c_2}\,t\right)\,e^{-w(x-\frac{c_3}{c_2}t)}$. It is clear that $G(x,t)$ is completely monotonic for all $x \geq \frac{c_3}{c_2}\,t$ as a composition of a completely monotonic function and an absolutely monotonic function (see Lemma 7.1, Chapter 7). Also, $G(x,t)$ vanishes to zero, as $x \to \infty$, since $w(s)$ satisfies conditions (H1-H3) above. Clearly, the function $F(x,t)$ is completely monotonic in $x \geq 0$. Indeed, one can calculate F_x and obtain

$$F_x(x,t) = -\frac{c_2}{c_3}\left\{1 - \frac{2\,c_2^2}{c_3^2}\,e^{-w\left(x-\frac{c_3}{c_2}t\right)}\right\}^{-1/2} w'\left(x - \frac{c_3}{c_2}\,t\right)e^{-w\left(x-\frac{c_3}{c_2}t\right)}$$

The function $-F_x$ is a product of two completely monotonic functions

$$f_3(x,t) := e^{-w\left(x-\frac{c_3}{c_2}t\right)}\,w'\left(x - \frac{c_3}{c_2}\,t\right) \quad \text{and} \quad f_1(x,t) = \left(1 - \frac{2\,c_2^2}{c_3^2}\,e^{-w\left(x-\frac{c_3}{c_2}t\right)}\right)^{-1/2}.$$

The function f_1 is a composition of an absolutely monotonic function $(1-f_2)^{-1/2}$ and a completely monotonic function $f_2 = e^{-w}$ and as a result f_1 is completely monotonic for all $x \geq 0$ (see Lemma 7.1 in Chapter 7) and thus our example is now complete. □

Examples of functions $w(s)$ satisfying conditions (H1-H3).

Two examples of functions $w(s)$ satisfying (H1-H3) are:

(a) $w(s) = s^\alpha$, where $\alpha \in (0,1]$.

(b) $w(s) = \ln(1 + (s+a)^\beta)$, where $a > 0$ arbitrary and $\beta \in (0,1]$.

For the purpose of illustrating an example of a similarity solution we consider here the first example and leave the second example for future work.

Example (a): Let $w(s) = s^{\alpha}$, $\alpha \in (0,1]$. It follows immediately that $w(s)$ satisfies (H1-H3) in Example 4.8. For simplicity, denote by

$$q := 2\,c_2^2/c_3^2$$

Then the initial condition (4.91) becomes $h(x) = \frac{c_3}{c_2}\left(1 - \sqrt{1 - q\,e^{-x^{\alpha}}}\right)$. Moreover, the similarity solution in this case takes the form

$$F(x,t) = \frac{c_3}{c_2}\left\{1 - \sqrt{1 - q\,e^{-(x-\frac{c_3}{c_2}t)^{\alpha}}}\right\},$$

whereas the function $G(x,t)$ becomes

$$G(x,t) = \alpha\left(x - \frac{c_3}{c_2}t\right)^{\alpha-1} e^{-(x-\frac{c_3}{c_2}t)^{\alpha}} \tag{4.94}$$

Our aim is to determine the solution $c(\lambda,t)$ to (4.2). This follows from the general formula

$$c(\lambda,t) = \frac{c_3\,e^{-\lambda Q(t)}}{c_2\,\lambda}\,\mathcal{L}^{-1}\left\{1 - \sqrt{1 - q\,e^{-(x-\frac{c_3}{c_2}t)^{\alpha}}}\right\}(\lambda,t)$$

where $Q(t)$ satisfies the I.V.P.

$$Q'(t) = \frac{c_3}{c_2}\left\{1 - \sqrt{1 - q\,e^{-(Q(t)-\frac{c_3}{c_2}t)^{\alpha}}}\right\} \quad \text{subject to I.C.} \quad Q(0) = 0. \tag{4.95}$$

Next, we make the assumption that $\alpha = 1$ and consider two different cases of study for q: Case 1: $q < 1$ and Case 2: $q = 1$ and determine whenever possible a formula for $Q(t)$ and $M_1(t)$ in both cases.

Case 1. Assume $q < 1$

If $q < 1$ then the differential equation (4.95) can be solved exactly as in this case it reduces to a separable differential equation whose solution is

$$Q(t) = \frac{c_3}{c_2}t + 2\,\ln\left(\frac{B^2\exp\left(-\frac{c_3}{2c_2}t\right) + q\exp\left(\frac{c_3}{2c_2}t\right)}{2B}\right) \text{ for } 0 \le t < T_c := \frac{c_2}{c_3}\,\ln\left(\frac{B^2}{q}\right). \tag{4.96}$$

where $B := 1 + \sqrt{1-q} > 0$.

Furthermore, we notice that for $t > T_c$, the function $Q(t) = \ln q + \frac{c_3}{c_2}t$ satisfies (4.95). Hence, we obtain the expression of $Q(t)$ for all time $t \geq 0$ in the form:

$$Q(t) = \begin{cases} 2\ln\left(\frac{B^2\exp\left(-\frac{c_3}{2c_2}t\right)+q\exp\left(\frac{c_3}{2c_2}t\right)}{2B}\right) + \frac{c_3}{c_2}t & \text{for} \quad 0 \leq t \leq T_c \\ \ln q + \frac{c_3}{c_2}t. & \text{for} \quad t > T_c \end{cases}$$

Moreover, the expression of the total mass in this case is obtained for all $t \geq 0$ from the definition $M_1(t) = Q'(t)$,

$$M_1(t) = \begin{cases} \frac{4c_2}{c_3}\frac{\exp\left(\frac{c_3}{2c_2}t\right)}{B^2\exp\left(-\frac{c_3}{2c_2}t\right)+q\exp\left(\frac{c_3}{2c_2}t\right)}, & \text{for} \quad 0 \leq t \leq T_c \\ \frac{c_3}{c_2}, & \text{for} \quad t > T_c \end{cases}$$

where $T_c = \frac{c_2}{c_3}\ln\left(\frac{B^2}{q}\right)$.

It remains only to show that T_c represents in fact the gel-time. This reduces to proving the following are true

$$M_1(t) = M_1(0) + \int_0^t \int_0^\infty \lambda\, g(\lambda, s)\, d\lambda\, ds \quad \text{for} \quad 0 \leq t < T_c \tag{4.97}$$

$$M_1(t) < M_1(0) + \int_0^t \int_0^\infty \lambda\, g(\lambda, s)\, d\lambda\, ds \quad \text{for} \quad t \geq T_c \tag{4.98}$$

Indeed, to show (4.97) holds, we calculate $M_1'(t)$ and $\int_0^\infty \lambda\, g(\lambda, t)\, d\lambda$. We have

$$\frac{dM_1(t)}{dt} = \frac{4B^2}{\left(B^2\exp\left(-\frac{c_3}{2c_2}t\right) + q\exp\left(\frac{c_3}{2c_2}t\right)\right)^2} \tag{4.99}$$

Moreover, using the definition of $\lambda\, g(\lambda, t)$ we obtain

$$\int_0^\infty \lambda\, g(\lambda, t)\, d\lambda = H(0,t) = G(Q(t), t) = e^{-(Q(t) - \frac{c_3}{c_2}t)} = e^{-v(t)} = \frac{dM_1(t)}{dt}$$

where $v(t) = Q(t) - \frac{c_3}{c_2}t$, from which (4.97) follows. Let us prove that (4.98) holds. Indeed, we have

$$E(t) := M_1(0) + \int_0^t \int_0^\infty \lambda\, g(\lambda, s)\, d\lambda\, ds = \frac{4c_2}{c_3(B^2+q)} + \int_0^t e^{-v(s)}\, ds$$

The last term of $E(t)$ is

$$\int_0^t e^{-v(s)}\,ds = \int_0^{T_c} e^{-v(s)}\,ds + \int_{T_c}^t e^{-v(s)}\,ds = I_1 + I_2$$

Using the expression of $v(s)$ we obtain that

$$I_1 = \int_0^{T_c} \frac{4\,B^2}{\left(B^2 \exp\left(-\frac{c_3}{2c_2}\,t\right) + q \exp\left(\frac{c_3}{2c_2}\,t\right)\right)^2}\,ds = \frac{c_2\,(B^2 - q)}{B\,q\,c_3} \quad \text{and}$$

$$I_2 = \int_{T_c}^t e^{-\ln q}\,ds = \frac{1}{q}\left[t - \frac{c_2}{c_3}\ln\left(\frac{B^2}{q}\right)\right]$$

Thus (4.98) holds if and only if

$$\frac{c_3}{c_2} \le \frac{1}{q}t - \frac{1}{q}\frac{c_2}{c_3}\ln\left(\frac{B^2}{q}\right) + \frac{2\,c_2}{q\,c_3} \quad \Leftrightarrow \quad \frac{c_3}{c_2} - \frac{2\,c_2}{q\,c_3} + \frac{T_c}{q} \le \frac{t}{q} \quad \Leftrightarrow \quad T_c \le t$$

where we used the definitions of T_c and q. Using (4.97) and (4.98) we can now conclude that $T_c \equiv T_{gel}$.

An explicit expression for the solution $c(\lambda, t)$ to the coagulation equation (4.2) requires the calculation of the inverse Laplace transform of $F(x, t)$ given by

$$F(x,t) = \frac{c_3}{c_2}\left\{1 - \sqrt{1 - q\,e^{-(x - \frac{c_3}{c_2}t)}}\right\} \quad \text{where} \quad q \le 1. \tag{4.100}$$

This can be obtained either by expanding the square root in (4.100) (using the binomial theorem) and then formally taking the inverse transform term by term or by directly computing the inverse Laplace transform of $F(x, t)$ in (4.100) with the help of contour integration. We leave the latter as future work. Next, we determine the asymptotic large size ($\lambda \to \infty$) solution.

Remark 4.7 *Case 2 (i.e. $q = 1$) is obtained from Case 1 in the limit as $q \to 1$.*

Asymptotic large size ($\lambda \to \infty$) behaviour of the solution (for $q \le 1$)

Based on the form of the similarity solution (4.100), we investigate the behaviour of $c(\lambda, t)$ for $\lambda \to \infty$, for $q \in (0, 1]$. For this reason, we return to the form of $F(x, t) = \frac{c_3}{c_2} + \psi(s)$ and apply the theory in [23] with regards to the image function $F(x, t)$. First, we need to determine the branch points $x_0(t)$ for $F(x, t)$ and find the asymptotic behaviour of $F(x,t)$ as $x \to x_0(t)$ for all times $t \geq 0$, by first determining the asymptotic behaviour of $\psi(s)$ as $s \to s_0$.

We have $\psi(s) = -\sqrt{2\,(k - e^{-s})}$, where $k = \frac{c_3^2}{2\,c_2^2} = \frac{1}{q}$. Then, the branch points for $\psi(s)$ are s_0 s.t. $k = e^{-s_0} \Rightarrow s_0 = -\ln(k) = \ln\left(\frac{2\,c_2^2}{c_3^2}\right)$. We can rewrite $\psi(s)$ as follows $\psi(s) = -\sqrt{2\,k}\,\sqrt{1 - e^{-(s-s_0)}} = -\frac{c_3}{c_2}\sqrt{1 - e^{-(s-s_0)}}$. We want to find a Puiseux series for $\psi(s)$ as $s \to s_0$. Using the MacLaurin series for e^{-x} we obtain $\psi(s) \sim -\frac{c_3}{c_2}\,(s - s_0)^{1/2} + \frac{c_3}{2\,c_2}\,(s - s_0)^{3/2} + \ldots$ as $s \to s_0$. In terms of $F(x,t)$, the asymptotic behaviour reads as

$$F(x,t) \sim \frac{c_3}{c_2} - \frac{c_3}{c_2}\,(x - x_0(t))^{1/2} + \frac{c_3}{2\,c_2}\,(x - x_0(t))^{3/2} + \ldots \quad \text{as} \quad x \to x_0(t)$$

where $x_0(t) = \frac{c_3}{c_2}\,t + \ln\left(\frac{2\,c_2^2}{c_3^2}\right)$ and t is fixed. Using [23] we obtain the asymptotic behaviour of $\lambda\, f(\lambda,t) = \mathcal{L}^{-1}\{F(x,t)\}(\lambda,t)$, as $\lambda \to \infty$, in the form

$$f(\lambda,t) \sim \frac{c_3}{2\,c_2\,\sqrt{\pi}}\,\lambda^{-5/2}\,e^{x_0(t)\,\lambda}, \quad \text{as} \quad \lambda \to \infty \text{ and for any } t \geq 0.$$

In addition, we also obtain the asymptotic behaviour of $c(\lambda,t)$ to be

$$c(\lambda,t) = e^{-\lambda\,Q(t)}\,f(\lambda,t) \sim e^{-\lambda\,(Q(t)-x_0(t))}\,\frac{c_3}{2\,c_2\,\sqrt{\pi}}\,\lambda^{-5/2}, \quad \text{as} \quad \lambda \to \infty, \text{ and for any } t \geq 0,$$

where $Q(t)$ is given in Case 1 and Case 2 above. Consequently, we have

Example 4.9 *Assume c_2, c_3 are some arbitrary constants such that $\frac{c_3}{c_2} \in (0, \sqrt{2}]$. Let $q = \frac{2\,c_2^2}{c_3^2}$ and $B := 1 + \sqrt{1-q} > 0$. Let the initial condition to the coagulation equation (4.2) be given by*

$$\lambda\,c_0(\lambda) = \frac{c_3}{c_2}\,\mathcal{L}^{-1}\left\{1 - \sqrt{1 - \frac{2\,c_2^2}{c_3^2}\,e^{-x}}\right\}(\lambda) \quad \left(so,\ c_0(\lambda) \sim \frac{c_3}{2\,c_2\,\sqrt{\pi}}\,\lambda^{-5/2}\,e^{-\lambda\ln\left(\frac{c_3^2}{2\,c_2^2}\right)}\right)$$

Let the function $Q(t)$ be given by

$$Q(t) = \begin{cases} 2\ln\left(\frac{B^2\exp\left(-\frac{c_3}{2\,c_2}\,t\right) + q\exp\left(\frac{c_3}{2\,c_2}\,t\right)}{2\,B}\right) + \frac{c_3}{c_2}\,t, & \text{for} \quad 0 \leq t \leq T_{gel} \\ \ln q + \frac{c_3}{c_2}\,t, & \text{for} \quad t > T_{gel} \end{cases}$$

where $T_{gel} = \frac{c_2}{c_3}\ln\left(\frac{B^2}{q}\right)$ denotes the gel-time. Assume the source function is such that $\lambda\,g(\lambda,t) = \delta(\lambda - 1)\,e^{-(Q(t)\,\lambda - \frac{c_3}{c_2}\,t)}$. Let the coagulation kernel be $K(\lambda,\mu) = \lambda\,\mu$. Then the asymptotic behaviour of the solution $c(\lambda,t)$ to the coagulation equation (4.2) is given by

$$c(\lambda,t) \sim \frac{c_3}{2\,c_2\,\sqrt{\pi}}\,\lambda^{-5/2}\,e^{-\lambda\,(Q(t) - \frac{c_3}{c_2}\,t - \ln q)}, \quad as \quad \lambda \to \infty, \text{ and } \forall t \geq 0. \qquad \square$$

4.2.4 Coagulation kernel $K(\lambda,\mu) = (\alpha+\beta\,\lambda)\,(\alpha+\beta\,\mu)$ and $g(\lambda,t)=0$

In this case, the PDE (4.10) reduces to

$$F_t(x,t)\,e^{\alpha\,Q(t)} + \beta\,F(x,t)\,F_x(x,t) = \frac{\alpha}{2}\,F^2(x,t). \tag{4.101}$$

Generators for the one-group of transformations

We determine the generators for the Lie group of point-transformations admitted by (4.101). In this case, equation (4.33) becomes

$$\begin{aligned} &2\,e^{\alpha\,Q(t)}\,Q'(t)\,F_1'(t) + \frac{2}{\alpha}\,e^{\alpha\,Q(t)}\,F_1''(t) \\ &\qquad + \frac{1}{3}\,e^{\frac{\alpha}{2\beta}x}\left\{F_2''(t) - \alpha\,Q''(t)\,F_2(t) - \alpha\,Q'(t)\,F_2'(t) + \frac{2\,F_3'(t)}{\beta}\right\} = 0 \end{aligned} \tag{4.102}$$

Since the coefficients of (4.102) are arbitrary functions of t then in order for (4.102) to hold for all values of $x \geq 0$ the following conditions for the functions $F_1(t)$, $F_2(t)$ and $F_3(t)$ must hold

$$F_1''(t) + \alpha\,Q'(t)\,F_1'(t) = 0 \quad \text{and} \quad F_2''(t) - \alpha\,\frac{d}{dt}\Big(F_2(t)\,Q'(t)\Big) + \frac{2}{\beta}\,F_3'(t) = 0 \tag{4.103}$$

from which we obtain the general solution in the form

$$F_1(t) = b_1\,R(t) + b_2 \quad \text{where} \quad R(t) = \int_0^t e^{-\alpha\,Q(s)}\,ds \tag{4.104}$$

where b_1 and b_2 are arbitrary constants. In addition, using (4.22) we have $C_t = 0$ and from the definition of $C(x,t)$ in (4.17) we obtain that the generator $\xi(x,t)$ satisfies the equation

$$\xi_{tt}(x,t) + \alpha\,Q'(t)\,\xi_t(x,t) = 0. \tag{4.105}$$

On the other hand, using (4.31) to calculate ξ_t and ξ_{tt}, (4.105) becomes

$$e^{-\frac{\alpha}{2\beta}x}\,R_1(t) + e^{\frac{\alpha}{2\beta}x}\,R_2(t) + R_3(t) = 0 \tag{4.106}$$

where

$$\begin{aligned} R_1(t) := -\frac{4\,\beta}{\alpha}\,e^{\alpha\,Q(t)}\,\Big\{&Q''(t)\,F_1'(t) + \alpha\,[Q'(t)]^2\,F_1'(t) + Q'(t)\,F_1''(t) + Q'(t)\,F_1''(t) \\ &+ \frac{1}{\alpha}\,F_1'''(t) + \alpha\,[Q'(t)]^2\,F_1'(t) + Q'(t)\,F_1''(t)\Big\} \end{aligned}$$

$$R_2(t) := F_4''(t) + \alpha\, Q'(t)\, F_4'(t) \quad \text{and} \quad R_3(t) := R_4'(t) + \alpha\, Q'(t)\, R_4(t)$$

$$R_4(t) := -\frac{2\beta}{\alpha}\left[F_2''(t) - \alpha\, Q''(t)\, F_2(t) - \alpha\, Q'(t)\, F_2'(t) + \frac{1}{\beta}\, F_3'(t)\right]$$

If we take the coefficient $R_1(t)$ of $e^{-\frac{\alpha}{2\beta}x}$ in (4.106) separately and use (4.104) we obtain

$$R_1(t) = \frac{4\beta\, b_1}{\alpha}\, e^{-\alpha\, Q(t)} \left\{Q''(t) - \alpha\,[Q'(t)]^2 + 3\,\alpha\,[Q'(t)]^2 - 2\,\alpha\,[Q'(t)]^2 - Q''(t)\right\} = 0$$

Hence, (4.106) becomes $e^{\frac{\alpha}{2\beta}x}\, R_2(t) + R_3(t) = 0$, from which when using (4.103) we obtain

$$F_4''(t) + \alpha\, Q'(t)\, F_4'(t) = 0 \quad \text{and} \quad F_3''(t) + \alpha\, Q'(t)\, F_3'(t) = 0. \tag{4.107}$$

Moreover, we also have

$$F_2''(t) - \alpha \frac{d}{dt}\Big[F_2(t)\, Q'(t)\Big] + \frac{2}{\beta}\, F_3'(t) = 0. \tag{4.108}$$

Therefore, the functions $F_i(t)$, with $i = 1, 2, 3, 4$ are given by

$$F_1(t) = b_1\, R(t) + b_2, \quad F_3(t) = a_1\, R(t) + a_2, \quad F_4(t) = a_3\, R(t) + a_4 \tag{4.109}$$

$$F_2(t) = e^{\alpha\, Q(t)} \left\{a_6 - \frac{2\, a_1}{\beta} \int^t R(t)\, e^{-\alpha\, Q(t)}\, dt + a_5\, R(t)\right\} \tag{4.110}$$

where $R(t) = \int_0^t e^{-\alpha\, Q(\tau)}\, d\tau$, and a_1, a_2, a_3, a_4, b_1 and b_2 are arbitrary constants. Substituting these functions into (4.29-4.32) and using the definition $\eta = A\, F^2 + B\, F + C$, we obtain

$$\zeta(x,t) = e^{\alpha\, Q(t)} \left\{\frac{2\, b_1}{\alpha}\, R(t)\, e^{-\frac{\alpha}{2\beta}x} + \frac{2\, b_2}{\alpha}\, e^{-\frac{\alpha}{2\beta}x} - \frac{a_1}{\beta}\, R^2(t) + a_5\, R(t) + a_6\right\} \tag{4.111}$$

$$\xi(x,t) = \frac{2\, a_1}{\alpha}\, R(t) + a_3\, e^{\frac{\alpha}{2\beta}x}\, R(t) + a_4\, e^{\frac{\alpha}{2\beta}x} - \frac{4\beta\, b_1}{\alpha^2}\, e^{-\frac{\alpha}{2\beta}x} - \left(\frac{2\, a_2}{\alpha} + \frac{2\beta\, a_5}{\alpha}\right) \tag{4.112}$$

$$\begin{aligned}\eta(x,t,F) = {} & a_1\left(\frac{2\, R(t)\, F}{\beta} + \frac{2}{\alpha\beta}\right) + a_3\, e^{\frac{\alpha}{2\beta}x}\left(\frac{\alpha\, R(t)\, F}{2\beta} + \frac{1}{\beta}\right) + a_4\, \frac{\alpha}{2\beta}\, e^{\frac{\alpha}{2\beta}x}\, F \\ & - a_5\, F + b_1\, R(t)\, F^2\, e^{-\frac{\alpha}{2\beta}x} + b_2\, F^2\, e^{-\frac{\alpha}{2\beta}x}\end{aligned} \tag{4.113}$$

If we denote by $c_1 = -a_5 - \frac{2}{\beta}\, a_2$; $c_2 = a_6$; $c_3 = a_4$; $c_4 = a_3$; $c_5 = -\frac{2}{\alpha}\, a_2 - \frac{2\beta}{\alpha}\, a_5$; $c_6 = \frac{2}{\alpha}\, a_1$; $c_7 = b_1$; $c_8 = b_2$ then the generators of the Lie group of point-transformations admitted by (4.101) are given by the following formulas

$$\begin{aligned}
\xi(x,t) &= c_3\, e^{\frac{\alpha}{2\beta}x} + c_4\, e^{\frac{\alpha}{2\beta}x}\, R(t) + c_5 + c_6\, R(t) - c_7\, \frac{4\beta}{\alpha^2}\, e^{\frac{-\alpha}{2\beta}x} \\
\zeta(x,t) &= c_1\, e^{\alpha Q(t)}\, R(t) + c_2\, e^{\alpha Q(t)} - c_5\, \frac{\alpha\, R(t)}{\beta}\, e^{\alpha Q(t)} - c_6\, \frac{\alpha\, R^2(t)}{2\,\beta}\, e^{\alpha Q(t)} \\
&+ c_7\, \frac{2\, R(t)}{\alpha}\, e^{-\frac{\alpha}{2\beta}x}\, e^{\alpha Q(t)} + c_8\, \frac{2}{\alpha}\, e^{-\frac{\alpha}{2\beta}x}\, e^{\alpha Q(t)} \\
\eta(x,t,F) &= -c_1\, F + c_3\, \frac{\alpha}{2\beta}\, e^{\frac{\alpha}{2\beta}x}\, F + c_4\, e^{\frac{\alpha}{2\beta}x}\left(\frac{\alpha}{2\beta}\, R(t)\, F + \frac{1}{\beta}\right) + c_5\, \frac{\alpha}{\beta}\, F \\
&+ c_6\left[\frac{\alpha}{\beta}\, R(t)\, F + \frac{1}{\beta}\right] + c_7\, R(t)\, F^2\, e^{-\frac{\alpha}{2\beta}x} + c_8\, F^2\, e^{-\frac{\alpha}{2\beta}x}
\end{aligned}$$

where $c_1, \dots, c_8$ are arbitrary constants (depending on $a_1, \dots, a_8$) and $R'(t) = e^{-\alpha Q(\tau)}\, d\tau$.

Therefore, the equation (4.101) has an eight-parameter Lie group of point transformations. More precisely, (4.101) admits an eight-dimensional Lie algebra $\mathcal{L}_8$ spanned by the following eight Lie symmetry vector fields $V_1, V_2, \dots, V_8$:

$$V_1 = e^{\alpha Q(t)}\, R(t) \frac{\partial}{\partial t} - F \frac{\partial}{\partial F}, \quad V_2 = e^{\alpha Q(t)} \frac{\partial}{\partial t}, \quad V_3 = e^{\frac{\alpha}{2\beta}x} \frac{\partial}{\partial x} + \frac{\alpha}{2\beta}\, e^{\frac{\alpha}{2\beta}x}\, F \frac{\partial}{\partial F}$$

$$\begin{aligned}
V_4 &= e^{\frac{\alpha}{2\beta}x}\, R(t)\, \frac{\partial}{\partial x} + e^{\frac{\alpha}{2\beta}x}\left[\frac{\alpha}{2\beta}\, R(t)\, F + \frac{1}{\beta}\right] \frac{\partial}{\partial F}, \quad V_5 = \frac{\partial}{\partial x} - \frac{\alpha}{\beta}\, e^{\alpha Q(t)}\, R(t) \frac{\partial}{\partial t} + \frac{\alpha}{\beta}\, F \frac{\partial}{\partial F} \\
V_6 &= R(t) \frac{\partial}{\partial x} - \frac{\alpha\, R^2(t)}{2\,\beta}\, e^{\alpha Q(t)} \frac{\partial}{\partial t} + \left[\frac{\alpha}{\beta}\, R(t)\, F + \frac{1}{\beta}\right] \frac{\partial}{\partial F} \\
V_7 &= -\frac{4\beta}{\alpha^2}\, e^{-\frac{\alpha}{2\beta}x} \frac{\partial}{\partial x} + \frac{2}{\alpha}\, R(t)\, e^{-\frac{\alpha}{2\beta}x}\, e^{\alpha Q(t)} \frac{\partial}{\partial t} + R(t)\, F^2\, e^{-\frac{\alpha}{2\beta}x} \frac{\partial}{\partial F} \\
V_8 &= \frac{2}{\alpha}\, e^{-\frac{\alpha}{2\beta}x}\, e^{\alpha Q(t)} \frac{\partial}{\partial t} + e^{-\frac{\alpha}{2\beta}x}\, F^2\, \frac{\partial}{\partial F}
\end{aligned} \tag{4.114}$$

Similar as in 4.2.2, we start by computing the commutator table and also the adjoint representation table. The commutator table for the Lie algebra arising from the infinitesimal generators V_i, where $i = 1, 2, \dots, 8$ is presented in Table 4.3.

$[V_i, V_j]$	V_1	V_2	V_3	V_4	V_5	V_6	V_7	V_8
V_1	0	$-V_2$	0	V_4	0	V_6	0	$-V_8$
V_2	V_2	0	0	V_3	$-\frac{\alpha V_2}{\beta}$	V_5	V_8	0
V_3	0	0	0	0	$-\frac{\alpha V_3}{2\beta}$	$-\frac{\alpha V_4}{2\beta}$	$\frac{3V_1}{\beta}+\frac{4V_5}{\alpha}$	$-\frac{V_2}{\beta}$
V_4	$-V_4$	$-V_3$	0	0	$\frac{\alpha V_4}{2\beta}$	0	$\frac{2V_6}{\alpha}$	$-\frac{3V_1}{\beta}-\frac{2V_5}{\alpha}$
V_5	0	$\frac{\alpha V_2}{\beta}$	$\frac{\alpha V_3}{2\beta}$	$-\frac{\alpha V_4}{2\beta}$	0	$-\frac{\alpha V_6}{\beta}$	$-\frac{\alpha V_7}{2\beta}$	$\frac{\alpha V_8}{2\beta}$
V_6	$-V_6$	$-V_5$	$\frac{\alpha V_4}{2\beta}$	0	$\frac{\alpha V_6}{\beta}$	0	0	$\frac{\alpha V_7}{2\beta}$
V_7	0	$-V_8$	$-\frac{3V_1}{\beta}-\frac{4V_5}{\alpha}$	$-\frac{2V_6}{\alpha}$	$\frac{\alpha V_7}{2\beta}$	0	0	0
V_8	V_8	0	$\frac{V_2}{\beta}$	$\frac{3V_1}{\beta}+\frac{2V_5}{\alpha}$	$-\frac{\alpha V_8}{2\beta}$	$-\frac{\alpha V_7}{2\beta}$	0	0

Table 4.3: Commutator $[V_i, V_j]$ table of (4.101) for the Lie algebra $\mathcal{L}_8$ spanned by V_i and V_j.

In the following we investigate the subalgebra structure for (4.114) of the PDE (4.101). In particular, we are interested in determining the optimal system of one-dimensional subalgebras of (4.101) and the corresponding invariant solutions. For this reason, we proceed similarly as in 4.2.2 and investigate the one-parameter group of adjoint transformations of the one-parameter subgroup $\exp(\varepsilon\, V_i)$ generated by the vector field V_i acting on the vector field V_j, where $i, j = 1, ..., 8$, defined by (4.43) (for more details about the adjoint representation and optimal systems see e.g. [80, 81]).

The corresponding adjoint representation structure for (4.114) can be easily constructed by using the formula (4.43) based on the infinitesimal generators given in the Table 4.3. The resulting operators are given in Table 7.2 in Chapter 7, where each (i, j)-th entry indicates $Ad(\exp(\varepsilon\, V_i))\, V_j$.

Following a similar analysis as in 4.2.2, we have obtained an optimal system of one-dimensional subalgebras. The proof of Theorem 4.4 below is presented in Chapter 7.

Theorem 4.4 *A one-dimensional optimal system of one-dimensional subalgebras of the full symmetry algebra for the PDE (4.101) is given by the following vector fields*

(i) $V_8+V_6+c_3\,V_3+c_2\,V_2+c_1\,V_1$; $V_8+V_4+c_1\,V_1$; $V_8+c_3\,V_3+c_1\,V_1$, $V_8+V_5+c_1^*\,V_1$, *(where* $c_1^* \neq \frac{\alpha}{\beta}$*) and* $V_8+V_5+\frac{\alpha}{\beta}\,V_1+c_2\,V_2$;

(ii) $V_7+V_2+c_4\,V_4+c_3\,V_3$, $V_7+V_2+V_1+c_6\,V_6+c_3\,V_3$, $V_7+c_5\,V_5+c_1\,V_1$, *and* $V_7+V_3+c_6\,V_6+c_5\,V_5$;

(iii) $V_6+V_2+c_1\,V_1$, $V_6+c_3\,V_3$, $V_6+V_1+c_3\,V_3$, $V_6+V_5+\frac{\alpha}{2\beta}\,V_1+c_4\,V_4$, $V_6+V_5+\bar{c}_1\,V_1$, *where* $\bar{c}_1 \neq \frac{\alpha}{2\beta}$;

(iv) $V_5 + c_1 V_1$, *where* $c_1 \neq \frac{\alpha}{\beta}, \frac{\alpha}{2\beta}$, *and* $V_5 + \frac{\alpha}{\beta} V_1 + c_2 V_2$;

(v) $V_4 + V_1 + c_2 V_2$, *and* $V_4 + c_2 V_2$;

(vi) $V_3 + c_2 V_2$, *and* $V_3 + c_1 V_1$;

(vii) $V_2 + c_1 V_1$;

(viii) V_1,

where $c_1, c_2, c_3, c_4, c_5, c_6, c_1^*, \bar{c}_1 \in \mathbb{R}$ *are arbitrary constants, with* c_1, c_1^*, $\bar{c}_1$ *subject to constants in (iv), (i) and (iii), respectively.*

According to the optimal system of one-dimensional subalgebras given in Theorem 4.4 of the full symmetry algebras of (4.101), it is possible to obtain the classification of all possible corresponding reduced forms of the partial differential equation (4.101). To illustrate some of the reductions forms of the PDE (4.101) we consider some of the vector fields in Theorem 4.4 and the corresponding similarity solutions $F(x,t)$:

(viii) $V = V_1$

$$F(x,t) = C_1(t)\, e^{\frac{\alpha}{2\beta}x} - \frac{2}{\alpha}, \quad \text{where } C_1(t) \text{ is an arbitrary function of } t.$$

(vii) $V = V_2 + m\, V_1$, where m is an arbitrary constant

$$F(x,t) = C_2(t)\, e^{\frac{\alpha}{2\beta}x} - \frac{2\beta m}{\alpha(1 + R(t))}, \quad \text{where } C_2(t) \text{ is an arbitrary function of } t.$$

(vi) $V = V_3 + \mu\, V_1$ where μ is an arbitrary constant

$$F(x,t) = e^{-W\left(-\beta\mu e^{-c\mu} e^{\frac{2\beta\mu}{\alpha} e^{-\frac{\alpha}{2\beta}x}} R(t)\right)} e^{-c\mu}\, e^{\frac{\alpha}{2\beta}x}\, e^{\frac{2\mu\beta}{\alpha} e^{-\frac{\alpha}{2\beta}x}}$$

where W is the Lambert W-function.

(v) $V = V_4 + \delta\, V_1$, where $\delta \neq 0$ is an arbitrary constant

$$F(x,t) = \frac{1}{\beta\,\delta}\, e^{\frac{\alpha}{2\beta}x} \quad \text{and} \quad F(x,t) = -\frac{2}{\alpha\, R(t)} - \frac{\alpha}{2\,\beta\,\delta\, R(t)}\, e^{\frac{\alpha}{2\beta}x} A.$$

Remark 4.8 *None of these similarity solutions obtained in the cases above satisfy the definition of F as a Laplace transform, and thus they are not of interest to our study.*

Vector field $V = V_5 + b\,V_1$

According to Theorem 4.4 (iv), the constant $b \neq \frac{\alpha}{\beta}, \frac{\alpha}{2\beta}$. In this case the generators of the Lie group of point transformations admitted by the PDE (4.101) take the form

$$\xi(x,t) = 1, \quad \zeta(x,t) = \left(b - \frac{\alpha}{\beta}\right) e^{\alpha\,Q(t)}\,R(t), \quad \eta(x,t,F) = -\left(b - \frac{\alpha}{\beta}\right) F.$$

Thus, the invariant surface condition (4.45) becomes a first order PDE

$$F_x + \left(b - \frac{\alpha}{\beta}\right) \frac{R(t)}{R'(t)}\,F_t = -\left(b - \frac{\alpha}{\beta}\right) F, \quad \text{where we used the definition: } R'(t) = e^{-\alpha\,Q(t)} \tag{4.115}$$

from which using the method of characteristics, we obtain the similarity solution and the similarity variable

$$F(x,t) = \psi(s)\,e^{\gamma x} \quad \text{and} \quad s \equiv -x - \frac{1}{\gamma}\,\ln[R(t)], \tag{4.116}$$

where $\gamma = \frac{\alpha - b\beta}{\beta}$. Substituting the invariant solution (4.116) into (4.101) we obtain that the similarity profile $\psi(s)$ satisfies the ODE

$$\psi'(s) = \frac{e^{-\gamma s}\,\psi^2(s)\,c_1}{1 + c_2\,e^{-\gamma s}\,\psi(s)} \tag{4.117}$$

whose solution is given by

$$\left[-\gamma\left(\frac{\alpha}{2}\,e^{-\gamma s}\,\psi(s) + 1\right)\right]^{\frac{2b\beta-\alpha}{\alpha}} = \psi(s)\,A_1 \tag{4.118}$$

where $c_1 = \frac{(b\beta-\alpha)(2\,b\beta-\alpha)}{2\beta}$ and $c_2 = \alpha - b\,\beta$ and A_1 is an arbitrary integration constant. Using the definitions of F and s in (4.116), we obtain $e^{-\gamma s} = e^{\gamma x}\,R(t)$, from which we can derive an algebraic equation for $F(x,t)$ in the form

$$\left[\frac{\alpha}{2}\,R(t)\,F(x,t) + 1\right]^{\frac{2b\beta-\alpha}{\alpha}} = e^{-\gamma x}\,F(x,t)\,A, \tag{4.119}$$

where $A = A_1\,(-\gamma)^{-\frac{2b\beta-\alpha}{\alpha}}$. In particular, if we take $t = 0$ we obtain that the initial condition to the PDE (4.101) for which a similarity solution as in (4.119) arise, is given by $h(x) = m\,e^{\gamma x}$, where we denote by $m := 1/A$. Based on the expression of $h(x)$ we obtain some necessary conditions for $h(x)$ to be completely monotonic in x and also to vanish to zero as $x \to \infty$. These conditions are $\gamma < 0$ and $m > 0$. The first condition implies that $b > \frac{\alpha}{\beta}$ (and thus the parameter b is strictly positive). Moreover if we denote by $\mu = \frac{2b\beta-\alpha}{\alpha}$ then the above condition yields $\mu > 1$. Therefore, we obtain the following result

Example 4.10 *Let* $\gamma := \frac{\alpha - b\beta}{\beta} < 0,\quad \mu = \frac{2b\beta - \alpha}{\alpha} > 1$ *and* $m = \frac{(-\gamma)^\mu}{A_1} > 0$.
Suppose the initial condition to (4.101) or (4.2) is

$$h(x) = m\, e^{\gamma x},\ \forall\, x \geq 0 \quad \left(so,\ \ c_0(\lambda) = \frac{m}{\alpha + \beta\lambda}\, \delta(\lambda + \gamma),\ \forall\, \lambda \geq 0\right)$$

Assume the coagulation kernel is $K(\lambda, \mu) = (\alpha + \beta\, \mu)\, (\alpha + \beta\, \lambda)$. *Let the source be* $g(\lambda, t) = 0$. *Then the solution* $c(\lambda, t)$ *of (4.2) has the form*

$$c(\lambda, t) = \frac{e^{-(\alpha + \beta\,\lambda)\, Q(t)}}{\alpha + \beta\lambda}\, \mathcal{L}^{-1}\{F(x, t)\}(\lambda, t)$$

where $F(x, t)$ *is the similarity solution of (4.101) and satisfies the equation*

$$m \left(\frac{\alpha}{2}\, R(t)\, F(x, t) + 1\right)^\mu = F(x, t)\, e^{-\gamma x} \tag{4.120}$$

and $Q(t)$ *satisfies the I.V.P.*

$$Q'(t) = e^{-\alpha\, Q(t)}\, F(\beta\, Q(t), t) \quad \textit{subject to} \quad I.C.\ Q(0) = 0. \tag{4.121}$$

Finding a general solution $F(x, t)$ for the equation (4.120) or the behaviour of the solution $c(\lambda, t)$ for a general constant $\mu > 1$ is not straightforward. An asymptotic behaviour of the solution $c(\lambda, t)$ based on the Newton polygon method can be applied in this case (see the similar analysis in 4.2.2). However, we restrict our attention to providing an expression for the total mass $M_1(t)$ of the solution $c(\lambda, t)$ to the coagulation equation (4.2) in the pre- and post-gelation regimes. We also determine the expression of the gelation time T_{gel} and the formula for $N(t)$ for all time $t \geq 0$.

We start by solving the I.V.P. (4.121) to determine the function $Q(t)$. Substituting $x = \beta Q(t)$ into (4.120) and using the definition of γ to get $\alpha - \gamma\beta = b\,\beta$ we obtain

$$m\left(\frac{\alpha}{2}\, R(t)\, e^{\alpha Q(t)}\, Q'(t) + 1\right)^\mu = e^{(\alpha - \gamma\,\beta)\, Q(t)}\, Q'(t) = e^{b\,\beta\, Q(t)}\, Q'(t)$$

Using the definition of $R(t)$, we rewrite the equation in the form

$$\frac{\alpha}{2}\, R(t) + \frac{e^{-\alpha\, Q(t)}}{Q'(t)} = \Big[Q'(t)\Big]^{\frac{1}{\mu} - 1}\, e^{\left(\frac{b\beta}{\mu} - \alpha\right) Q(t)} \left(\frac{1}{m}\right)^{1/\mu}$$

Next, we take the derivative w.r.t t on both sides. Multiplying the result by $2\,[Q'(t)]^2$ and using the definition of μ, we obtain

$$\left\{\alpha\, [Q'(t)]^2 + 2\, Q''(t)\right\} \left\{e^{-\alpha\, Q(t)} + 2 \left(\frac{Q'(t)}{m}\right)^{1/\mu} \frac{\alpha - b\,\beta}{2\,b\,\beta - \alpha}\, e^{\frac{\alpha\,(\alpha - b\,\beta)}{2\,b\,\beta - \alpha}\, Q(t)}\right\} = 0. \tag{4.122}$$

In the absence of particle source terms and since c_0 has a finite second moment, it is expected that prior to the occurrence of a shock (gelation) the total mass be conserved, i.e.

$$M_1(t) = M_1(0) = \int_0^\infty \lambda\, c_0(\lambda)\, d\lambda = \frac{m(b\beta - \alpha)}{b\beta^2} \quad \text{for} \quad t \in [0, T_{gel}).$$

In addition, in this case, the function $N(t)$ satisfies the I.V.P.

$$N'(t) = -\frac{\alpha}{2} N^2(t) \quad \text{subject to I.C} \quad N(0) = h(0) = m > 0, \tag{4.123}$$

(see for example [96]). The shock/gel time T_{gel} is still unknown at this stage and needs to be determined. On the other hand, using the definition $N(t) = Q'(t)$, the equation (4.123) takes the form

$$Q''(t) = -\frac{\alpha}{2} [Q'(t)]^2 \quad \Rightarrow \quad \alpha [Q'(t)]^2 + 2\, Q''(t) = 0, \quad \text{for } t \in [0, T_{gel})$$

(which corresponds to the first factor in (4.122)). One can solve the equation (4.123) and obtain an expression for $N(t)$ prior to the occurrence of gelation:

$$Q'(t) = N(t) = \frac{2\, h(0)}{2 + \alpha\, h(0)\, t} \quad \Rightarrow \quad N(t) = \frac{2\, m}{2 + \alpha\, m\, t} \quad \text{for} \quad t \in [0, T_{gel}).$$

Moreover, we also obtain an expression for $Q(t)$ in this case to be

$$Q(t) = \frac{2}{\alpha} \ln\left(\frac{2 + \alpha\, m\, t}{2}\right) \quad \text{for} \quad t \in [0, T_{gel}). \tag{4.124}$$

For the expression of T_{gel} we use the same definition in [96] which corresponds to the instance when $M_2(t) = F_x(Q(t), t) \to -\infty$, or

$$T_{gel} = -\frac{1}{\beta\, h'(0^+)} = -\frac{1}{\beta . m\, \gamma} = \frac{1}{m\,(b\beta - \alpha)} > 0. \tag{4.125}$$

After the occurrence of a shock (so, for $t \geq T_{gel}$), it is expected that the equation $2\, Q''(t) + \alpha\, Q'(t)^2 = 0$ is no longer valid. According to the equation (4.122) for $Q(t)$ this means that in the post-gelation regime we have

$$e^{-\alpha Q(t)} + 2 \left(\frac{Q'(t)}{m}\right)^{1/\mu} \frac{\alpha - b\beta}{2\, b\beta - \alpha}\, e^{\frac{\alpha(\alpha - b\beta)}{2b\beta - \alpha} Q(t)} = 0.$$

Therefore, for $t \geq T_{gel}$, we have

$$Q'(t) = \frac{m}{2^\mu} \left(\frac{\alpha - 2\, b\beta}{\alpha - b\beta}\right)^\mu e^{-\frac{\alpha b\beta\mu}{2b\beta - \alpha} Q(t)}$$

Using the definition of μ we get that $\frac{\alpha b \beta \mu}{2b\beta - \alpha} = b\beta$ and thus the above equation simplifies to

$$Q'(t) = \frac{m}{2^\mu}\left(\frac{\alpha - 2b\beta}{\alpha - b\beta}\right)^\mu e^{-b\beta Q(t)} \quad \Rightarrow \quad Q'(t)\, e^{b\beta Q(t)} = \frac{m}{2^\mu}\left(\frac{\alpha - 2b\beta}{\alpha - b\beta}\right)^\mu \tag{4.126}$$

Integrating (4.126) from T_{gel} to t we obtain

$$e^{b\beta Q(t)} = e^{b\beta Q(T_{gel})} + \frac{m b\beta}{2^\mu}\left(\frac{\alpha - 2b\beta}{\alpha - b\beta}\right)^{\frac{2b\beta - \alpha}{\alpha}} (t - T_{gel}). \tag{4.127}$$

For the expression of $Q(T_{gel})$ we use the formula obtained for $Q(t)$ in the pre-gelation stage, ensuring the continuity of $M_1(t)$ and thus of $Q(t)$ and $c(\lambda, t)$ at $t = T_{gel}$. Using the definition of T_{gel} and the expression (4.124) we obtain

$$Q(T_{gel}) = \frac{2}{\alpha} \ln\left(\frac{2b\beta - \alpha}{2(b\beta - \alpha)}\right)$$

Then (4.127) becomes

$$e^{b\beta Q(t)} = t\, m\, b\beta \left(\frac{2b\beta - \alpha}{2(b\beta - \alpha)}\right)^{(2b\beta/\alpha)-1} - \frac{\alpha\,(2b\beta - \alpha)^{(2b\beta/\alpha)-1}}{\left[2\,(b\beta - \alpha)\right]^{2b\beta/\alpha}} \tag{4.128}$$

So,

$$Q(t) = \frac{1}{b\beta} \ln\left\{\left[\frac{2b\beta - \alpha}{2(b\beta - \alpha)}\right]^{(2b\beta/\alpha)-1} \left(mb\beta t - \frac{\alpha}{2(b\beta - \alpha)}\right)\right\} \tag{4.129}$$

Therefore we obtain the formula for $Q(t)$ for all $t \geq 0$ as

$$Q(t) = \begin{cases} \frac{2}{\alpha} \ln\left(\frac{2 + \alpha m t}{2}\right), & \text{for} \quad t \in [0, T_{gel}) \\ \frac{1}{b\beta} \ln\left\{\left[\frac{2b\beta - \alpha}{2(b\beta - \alpha)}\right]^{(2b\beta/\alpha)-1} \left(mb\beta t - \frac{\alpha}{2(b\beta - \alpha)}\right)\right\}, & \text{for} \quad t \geq T_{gel} \end{cases} \tag{4.130}$$

where T_{gel} represents the gel (shock)-time and is given by (4.125). From this formula one easily obtains the expression for $N(t) = Q'(t)$ for all $t \geq 0$

$$N(t) = \begin{cases} \frac{2m}{2 + \alpha m t} & \text{for} \quad t \in [0, T_{gel}) \\ \frac{2m(b\beta - \alpha)}{2b\beta m(b\beta - \alpha)t - \alpha} & \text{for} \quad t \geq T_{gel} \end{cases}$$

On the other hand, we make use of the definition of $N(t)$ as a linear combination of the zeroth and first moments, or

$$N(t) = \alpha\, M_0(t) + \beta\, M_1(t). \tag{4.131}$$

Since we only know the expression of the total mass $M_1(t)$ in the pre-gel stage we can determine the zeroth moment from the above equality. So, $M_0(t) = \frac{1}{\alpha}\Big\{N(t) - \beta\, M_1(t)\Big\}$, for $t \in [0, T_{gel})$, takes the form

$$M_0(t) = \frac{2m}{\alpha(2+\alpha m\, t)} - \frac{m(b\beta-\alpha)}{\alpha b\beta} = \frac{m(\alpha mt + 2 - b\beta mt)}{b\beta(2+\alpha mt)}, \quad \text{for } \ t \in [0, T_{gel}).$$

To determine the expression of $M_1(t)$ for $t \geq T_{gel}$ we need to find the zeroth moment for $t \geq T_{gel}$. For this purpose, integrate (4.2) w.r.t. x on $[0, \infty)$ and use the definitions of $M_0(t)$ and $M_1(t)$. Thus we obtain that the zeroth moment satisfies the I.V.P.

$$M_0'(t) = -\frac{1}{2}\, N^2(t), \quad \text{for all} \quad t \geq 0. \tag{4.132}$$

It remains only to determine $M_0(t)$ in the post-gelation regime. For this stage, we solve the ODE above and impose the initial condition $M_0(T_{gel})$ such that the function $M_0(t)$ is continuous at $t = T_{gel}$. Therefore, we need to solve the I.V.P. (4.132) subject to $M_0(T_{gel}) = \frac{m(b\beta-\alpha)}{b\beta(2\,b\beta-\alpha)}$. Integrating (4.132) from T_{gel} to t we obtain

$$\begin{aligned} M_0(t) = M_0(T_{gel}) - \frac{1}{2}\int_{T_{gel}}^{t} N^2(s)\, ds &= \frac{m}{2b\beta\Big(mb\beta t - \frac{\alpha}{2(b\beta-\alpha)}\Big)}\Bigg]_{T_{gel}}^{t} + \frac{m(b\beta-\alpha)}{b\beta(2\,b\beta-\alpha)} \\ &= \frac{m}{2\,b\beta-\alpha}\left\{\frac{b\beta-\alpha}{b\beta} - \frac{m(b\beta-\alpha)t-1}{mb\beta t - \frac{\alpha}{2(b\beta-\alpha)}}\right\} = \frac{m(b\beta-\alpha)}{b\beta\Big[2(b\beta-\alpha)mb\beta t - \alpha\Big]}, \end{aligned}$$

for $t \geq T_{gel}$. Substituting $M_0(t)$ above into (4.131) we obtain the expression of the first moment

$$M_1(t) = \frac{m(b\beta-\alpha)(2b\beta-\alpha)}{b\beta^2\Big[2(b\beta-\alpha)mb\beta t - \alpha\Big]} \quad \text{for} \quad t \geq T_{gel}$$

Therefore, we have obtained the expression of the total mass for all time $t \geq 0$

$$M_1(t) = \begin{cases} \frac{m(b\,\beta-\alpha)}{b\,\beta^2} & \text{for} \quad t \in [0, T_{gel}) \\ \frac{m(b\beta-\alpha)(2b\beta-\alpha)}{b\beta^2\Big[2(b\beta-\alpha)mb\beta t-\alpha\Big]} & \text{for} \quad t \geq T_{gel} \end{cases}$$

where T_{gel} represents the gelation time defined by (4.125). □

Particular choice of constants. Asymptotic and formal series solutions

In particular, if $\mu = 2$ then $b = \frac{3\alpha}{2\beta}$ and $\gamma = -\frac{\alpha}{2\beta}$. Moreover, in this case the algebraic equation (4.119) becomes quadratic and we obtain an explicit formula for $F(x,t)$

$$F(x,t) = \frac{2}{\alpha^2\, m\, R^2(t)} \left\{ e^{\frac{\alpha}{2\beta}x} - \alpha\, m\, R(t) - \sqrt{\left(e^{\frac{\alpha}{2\beta}x} - \alpha\, m\, R(t)\right)^2 - \left(\alpha\, m\, R(t)\right)^2} \right\} \tag{4.133}$$

The function $F(x,t)$ is completely monotonic for all $x \geq 0$. In addition, $F(x,t)$ has a branch point

$$x_0 = x_0(t) = \frac{2\beta}{\alpha} \ln(2\alpha m R(t)).$$

Expanding $F(x,t)$ about the branch point $x_0(t)$ we obtain the asymptotic behaviour of $F(x,t)$ as $x \to x_0(t)$ to be

$$F(x,t) \sim \frac{2}{m\alpha^2 R^2(t)} \left\{ \alpha m R(t) - 2\,\alpha m R(t) \sqrt{\frac{\alpha}{2\beta}} \left(x - \frac{2\,\beta}{\alpha} \ln(2\alpha m R(t)) \right)^{1/2} + \ldots \right\}$$

Therefore, according to [23] we obtain the asymptotic behaviour of the solution $f(\lambda,t)$ as $\lambda \to \infty$ to be

$$(\alpha + \beta\lambda)\, f(\lambda,t) \sim \frac{2}{m\alpha^2 R^2(t)} \left(- \frac{2\alpha\, m R(t)\, \lambda^{-3/2} \sqrt{\frac{\alpha}{2\beta}}}{\Gamma(-\frac{1}{2})} \right) e^{\frac{2\beta}{\alpha} \ln(2\alpha m R(t))\,\lambda}.$$

Using the definition of $c(\lambda,t)$ we obtain the asymptotic behaviour for the solution $c(\lambda,t)$ of (4.2) as $\lambda \to \infty$ for all $t \geq 0$ to be

$$c(\lambda,t) \sim \frac{\lambda^{-3/2}\, e^{-(\alpha+\beta\lambda)\,Q(t)}}{(\alpha + \beta\lambda)\, \alpha\, R(t)} \sqrt{\frac{2\,\alpha}{\beta\pi}} \left[2\alpha R(t)\, m \right]^{\frac{2\beta}{\alpha}\lambda} \quad \text{as} \quad \lambda \to \infty, \quad \forall t \geq 0 \tag{4.134}$$

where $Q(t)$ is obtained in (4.130) where we substitute $b\,\beta = 3\alpha/2$, so

$$Q(t) = \begin{cases} \frac{2}{\alpha} \ln\left(\frac{2+\alpha m t}{2}\right), & \text{for} \quad t \in [0, T_{gel}) \\ \frac{2}{3\alpha} \ln(6\alpha m t - 4), & \text{for} \quad t \geq T_{gel} = \frac{2}{\alpha m} \end{cases} \tag{4.135}$$

Alternatively, we can proceed as in Example 4.9 and expand the square root in $F(x,t)$ defined by (4.133) using the binomial theorem (or the Newton's generalized binomial theorem), and then formally take the inverse Laplace transform term by term to obtain the inverse Laplace transform of $F(x,t)$:

$$\begin{aligned}\mathcal{L}^{-1}\{F(x,t)\}(\lambda,t) &= 8m \sum_{k=2}^{\infty} (-1)^{k+1} \binom{1/2}{k} \left[2\alpha m R(t)\right]^{k-2} \delta\Big(\lambda - \frac{\alpha\,(k-1)}{2\beta}\Big) \\ &= 8m \sum_{k=2}^{\infty} \frac{(2k-2)!}{2^{2k-1} k!(k-1)!} \left[2\alpha m R(t)\right]^{k-2} \delta\Big(\lambda - \frac{\alpha\,(k-1)}{2\beta}\Big)\end{aligned}$$

Thus, the solution $c(\lambda,t)$ of the coagulation equation becomes

$$c(\lambda,t) = \frac{8\,m\,e^{-(\alpha+\beta\lambda)\,Q(t)}}{\alpha+\beta\lambda} \sum_{k=2}^{\infty} \frac{(2k-2)!}{2^{2k-1} k!(k-1)!} \left[2\alpha m R(t)\right]^{k-2} \delta\Big(\lambda - \frac{\alpha\,(k-1)}{2\beta}\Big)$$

and the initial condition is given by $c_0(\lambda) = \frac{m}{\alpha+\beta\,\lambda}\,\delta\Big(\lambda - \frac{\alpha}{2\beta}\Big)$. In this case, the expression of the total mass becomes:

$$M_1(t) = \begin{cases} \frac{m}{3\beta} & \text{for} \quad t \in [0, T_{gel}) \\ \frac{4\,m}{3\,\beta\,(3\,\alpha\,m\,t-2)} & \text{for} \quad t \geq T_{gel} = \frac{2}{\alpha\,m} \end{cases}$$

4.2.5 Coagulation kernel $K(\lambda,\mu) = (\alpha+\beta\,\lambda)\,(\alpha+\beta\,\mu)$ and $g(\lambda,t) > 0$

In this case, the PDE is given by the general form

$$F_t(x,t)\,e^{\alpha Q(t)} + \beta\,F(x,t)\,F_x(x,t) = \frac{\alpha}{2}\,F^2(x,t) + e^{\alpha Q(t)}\,G(x,t) \tag{4.136}$$

Generators for the one-group of transformations

In this case, since $\alpha > 0$, then from 4.2.1 the function $F_1(t) = 0$. Thus, the functions $A(x,t)$ and $\zeta(x,t)$ defined in (4.29) become $A(x,t) = 0$ and thus

$$\zeta(x,t) = F_2(t), \tag{4.137}$$

where $F_2(t)$ is an arbitrary function of t. Moreover, we have $\eta(x,t,F) = B(x,t)\,F + C(x,t)$, and (4.30) and (4.32) take the form

$$B(x,t) = \frac{\alpha}{2\,\beta}\,e^{\frac{\alpha}{2\beta}\,x}\,F_4(t) - (F_2'(t) - \alpha\,Q'(t)\,F_2(t)) \tag{4.138}$$

$$C(x,t) = \frac{1}{\beta}\,e^{\alpha\,Q(t)}\,F_4'(t)\,e^{\frac{\alpha}{2\beta}\,x} - \frac{2}{\alpha}\,e^{\alpha\,Q(t)} \left\{F_2'''(t) - \alpha\,Q''(t)\,F_2(t) - \alpha\,Q'(t)\,F_2'(t) + \frac{F_3'(t)}{\beta}\right\} \tag{4.139}$$

where $F_3(t)$ and $F_4(t)$ are arbitrary functions of t. Furthermore, using $F_1(t) = 0$ equation (4.33) gives rise to

$$F_2''(t) - \alpha\, Q''(t)\, F_2(t) - \alpha\, Q'(t)\, F_2'(t) = -\frac{2}{\beta}\, F_3'(t) \tag{4.140}$$

which by integration w.r.t. t twice yields

$$F_2(t) = -\frac{2}{\beta}\, e^{\alpha\, Q(t)} \int F_3(t)\, e^{-\alpha\, Q(t)}\, dt + a_1 e^{\alpha\, Q(t)} \int e^{-\alpha\, Q(t)}\, dt + c_1\, e^{\alpha\, Q(t)} \tag{4.141}$$

where a_1, c_1 are arbitrary constants of integration. Combining the formulas (4.139) and (4.140) we obtain

$$C(x,t) = \frac{1}{\beta}\, e^{\alpha\, Q(t)} \left\{ F_4'(t)\, e^{\frac{\alpha}{2\beta}x} + \frac{2}{\alpha}\, F_3'(t) \right\}. \tag{4.142}$$

On the other hand, since $C(x,t) = \frac{1}{\beta}\, e^{\alpha\, Q(t)}\, \xi_t(x,t)$, we obtain $\xi_t(x,t) = F_4'(t)\, e^{\frac{\alpha}{2\beta}x} + \frac{2}{\alpha}\, F_3'(t)$, which by integration w.r.t t gives us

$$\xi(x,t) = F_4(t)\, e^{\frac{\alpha}{2\beta}x} + \frac{2}{\alpha}\, F_3(t) + A_2(x), \tag{4.143}$$

where $A_2(x)$ is an arbitrary function of x. In addition, substituting the expression of $F_2(t)$ obtained in (4.141) into (4.138) we obtain

$$B(x,t) = \frac{\alpha}{2\beta}\, e^{\frac{\alpha}{2\beta}x}\, F_4(t) + \frac{2}{\beta}\, F_3(t) - a_1.$$

Furthermore, using the expressions of $B(x,t)$ and $C(x,t)$ obtained above we also determine the infinitesimal generator $\eta(x,t,F) = B(x,t)\, F + C(x,t)$ to be

$$\eta(x,t,F) = \left\{ \frac{\alpha}{2\beta}\, e^{\frac{\alpha}{2\beta}x}\, F_4(t) + \frac{2}{\beta}\, F_3(t) - a_1 \right\} F + \frac{1}{\beta}\, e^{\alpha\, Q(t)} \left\{ F_4'(t)\, e^{\frac{\alpha}{2\beta}x} + \frac{2}{\alpha}\, F_3'(t) \right\} \tag{4.144}$$

Therefore, the generators of the Lie group of transformations admitted by the PDE (4.136) are given by the equations (4.143), (4.137), and (4.144). With the help of these expressions we can proceed to determine the group-invariant or similarity solutions $F(x,t)$ of the PDE (4.136). Such similarity solutions are obtained by solving the invariant surface condition (4.45). Thus we obtain a first order linear PDE for $F(x,t)$

$$\begin{aligned} &\left[F_4(t)\, e^{\frac{\alpha}{2\beta}x} + \frac{2}{\alpha}\, F_3(t) + A_2(x) \right] F_x(x,t) + F_2(t)\, F_t(x,t) \\ &= \left[\frac{\alpha}{2\beta}\, e^{\frac{\alpha}{2\beta}x}\, F_4(t) + \frac{2}{\beta}\, F_3(t) - a_1 \right] F(x,t) + \frac{1}{\beta}\, e^{\alpha\, Q(t)} \left[F_4'(t)\, e^{\frac{\alpha}{2\beta}x} + \frac{2}{\alpha}\, F_3'(t) \right]. \end{aligned} \tag{4.145}$$

To illustrate our analysis in this case we only consider below the particular case $A_2(x) = a_2$, where a_2 is an arbitrary constant and $F_2(t) \neq 0$. The general case, $A_2(x)$ arbitrary function of x is left for future work.

From the invariant surface condition (4.145) we obtain

$$\begin{aligned} F_x + \frac{F_2(t)}{F_4(t)\, e^{\frac{\alpha}{2\beta}x} + \frac{2}{\alpha} F_3(t) + a_2} F_t &= \frac{\frac{\alpha}{2\beta} e^{\frac{\alpha}{2\beta}x} + \frac{2}{\beta} F_3(t) - a_1}{F_4(t)\, e^{\frac{\alpha}{2\beta}x} + \frac{2}{\alpha} F_3(t) + a_2} F \\ &+ \frac{e^{\frac{\alpha}{2\beta}x} F_4'(t)}{F_4(t)\, e^{\frac{\alpha}{2\beta}x} + \frac{2}{\alpha} F_3(t) + a_2} + \frac{2}{\alpha} \frac{F_3'(t)}{F_4(t) e^{\frac{\alpha}{2\beta}x} + \frac{2}{\alpha} F_3(t) + a_2} \end{aligned} \tag{4.146}$$

Using the definition of $F(x,t)$ we have $F_x \to 0$ as $x \to \infty$, then taking the limit $\lim_{x\to\infty}$ of (4.146) we obtain that a necessary condition for the new equality to hold for all $t \geq 0$ is that the function $F_4(t)$ is a constant. Indeed, assume first that $F_4(t) \neq 0$, then taking the limit in (4.146) as $x \to \infty$ we obtain that the left hand-side approaches zero while the right hand-side tends to $F_4'(t)/F_4(t)$. Therefore, $F_4'(t) = 0$, i.e. $F_4(t) = a_3$ is a constant. On the other hand, if $F_4(t) = 0$ then taking $\lim_{x\to\infty}$ of (4.146), the equality holds for all $t \geq 0$ if $F_3'(t) = 0$ which means that $F_3(t) = a_4$ is an arbitrary constant.

Therefore, the generators of the one-group of point transformations that leave the PDE (4.136) invariant take the following form

$$\begin{aligned} \xi(x,t) &= a_3\, e^{\frac{\alpha}{2\beta}x} + \frac{2}{\alpha} F_3(t) + a_2 \\ \zeta(x,t) &= F_2(t) = -\frac{2}{\beta} e^{\alpha Q(t)} \int F_3(t)\, e^{-\alpha Q(t)}\, dt + a_1\, e^{\alpha Q(t)} \int e^{-\alpha Q(t)}\, dt + a_5\, e^{\alpha Q(t)} \\ \eta(x,t,F) &= \left\{\frac{\alpha}{2\beta} e^{\frac{\alpha}{2\beta}x} a_3 + \frac{2}{\beta} F_3(t) - a_1\right\} F + \frac{2}{\alpha\beta} e^{\alpha Q(t)} F_3'(t) \end{aligned}$$

where we use the notation $a_5 := c_1$. In addition, from (4.22) the generators satisfy the following equality

$$\begin{aligned} &\left[a_3\, e^{\frac{\alpha}{2\beta}x} + \frac{2}{\alpha} F_3(t) + a_2\right] G_x(x,t) + F_2(t)\, G_t(x,t) \\ &\qquad = -G\left[F_2'(t) - \frac{\alpha}{2\beta} e^{\frac{\alpha}{2\beta}x} a_3 - \frac{2}{\beta} F_3(t) + a_1\right] + \frac{2}{\alpha} F_3''(t) \end{aligned} \tag{4.147}$$

where $G(x,t)$ is a completely monotonic function for all $x \geq 0$ such that its inverse Laplace transform exists and the arbitrary functions F_2, F_3, F_4 satisfy one of the following

(i) $F_4(t) = a_3 \neq 0$ arbitrary number and $F_3(t)$ arbitrary function of t.

(ii) $F_4(t) = 0$ and $F_3(t) = a_4$.

In both cases above, the function $F_2(t)$ is determined using the formula (4.141).

In the case (i), the invariant surface condition (4.145) takes the form

$$\begin{aligned}\Big(a_3 e^{\frac{\alpha}{2\beta}x} + \frac{2F_3(t)}{\alpha} + a_2\Big) F_x(x,t) + e^{\alpha Q(t)}\Big(-\frac{2}{\beta}\int F_3(t) e^{-\alpha Q(t)} dt + a_1\, R(t) + a_5\Big) F_t(x,t) \\ = \Big(\frac{\alpha}{2\beta} e^{\frac{\alpha}{2\beta}x} a_3 + \frac{2F_3(t)}{\beta} - a_1\Big)\, F(x,t) \qquad (4.148)\end{aligned}$$

where $F_3(t)$ is an arbitrary function of t, unknown at this point, yet to be determined, such that (4.147) holds. To obtain $F_3(t)$, one can consider a few examples of functions $G(x,t)$ and solve the equation (4.147), use being made of the formula (4.141), to find $F_2(t)$ thus obtaining the function $F_3(t)$. Using the formulas for the functions $F_i(t)$, $(i = 2,3,4)$ above one then solves the PDE (4.148) and thus obtains the similarity solutions. However, we leave this approach for future work.

In the following we present an example of a similarity solution $F(x,t)$ that we obtain in the second case (ii) above. In this case, since $F_3(t) = a_4$ and $F_4(t) = 0$ and using (4.141), we obtain

$$F_2(t) = \Big\{\Big(a_1 - \frac{2\,a_4}{\beta}\Big)\, R(t) + a_5\Big\}\, e^{\alpha Q(t)} \quad \text{where} \quad R(t) = \int_0^t e^{-\alpha Q(\tau)}\, d\tau. \qquad (4.149)$$

Therefore, the generators of the one-group of transformations that leave the PDE (4.136) invariant become

$$\begin{aligned}&\xi(x,t) = a_2 + \frac{2}{\alpha}\, a_4, \quad \zeta(x,t) = a_1\, R(t)\, e^{\alpha\, Q(t)} - \frac{2\,a_4}{\beta}\, R(t)\, e^{\alpha\, Q(t)} + a_5\, e^{\alpha\, Q(t)}, \\ &\eta(x,t,F) = -(a_1 - \frac{2}{\beta}\, a_4)\, F. \qquad (4.150)\end{aligned}$$

Next, substituting the functions F_2, F_3, F_4 above into the PDE (4.147) we can determine the form of the function $G(x,t)$, solution to (4.147)

$$\begin{aligned}\Big(\frac{2\,a_4}{\alpha} + a_2\Big) G_x(x,t) + \Big\{\Big(a_1 - \frac{2\,a_4}{\beta}\Big)\, R(t) + a_5\Big\}\, e^{\alpha\, Q(t)}\, G_t(x,t) \\ = -\Big\{2\,\Big(a_1 - \frac{2\,a_4}{\beta}\Big) + \alpha\, Q'(t)\, e^{\alpha\, Q(t)}\Big[\Big(a_1 - \frac{2\,a_4}{\beta}\Big)\, R(t) + a_5\Big]\Big\}\, G(x,t) \quad (4.151)\end{aligned}$$

Moreover, in this case the invariant surface condition (4.145) takes the following form

$$\left(\frac{2\,a_4}{\alpha}+a_2\right)F_x(x,t)+\left\{\left(a_1-\frac{2\,a_4}{\beta}\right)R(t)+a_5\right\}e^{\alpha\,Q(t)}\,F_t(x,t)=\left(\frac{2\,a_4}{\beta}-a_1\right)F(x,t) \tag{4.152}$$

The infinitesimal generator X associated to the above Lie group of transformations can be written as

$$V=a_1\,V_1+a_2\,V_2+a_4\,V_3+a_5\,V_4$$

where the vector fields are given by

$$V_1=e^{\alpha\,Q(t)}\,R(t)\frac{\partial}{\partial t}-F\,\frac{\partial}{\partial F},\quad V_2=\frac{\partial}{\partial x},\quad V_3=\frac{2}{\alpha}\,\frac{\partial}{\partial x}-\frac{2}{\beta}\,R(t)\,e^{\alpha\,Q(t)}\,\frac{\partial}{\partial t}+\frac{2}{\beta}\,F\,\frac{\partial}{\partial F},$$
$$V_4=e^{\alpha\,Q(t)}\,\frac{\partial}{\partial t} \tag{4.153}$$

These operators form a basis for the corresponding Lie algebra $\tilde{\mathcal{L}}_4$. The commutator table for the Lie algebra arising from the infinitesimal generators V_i, where $i=1,2,3,4$ is presented in Table 4.4. In addition, the corresponding adjoint representation structure for (4.153) can be easily constructed by using the formula (4.43) based on the infinitesimal generators given in the Table 4.4.

$[V_i,V_j]$	V_1	V_2	V_3	V_4
V_1	0	0	0	$-V_4$
V_2	0	0	0	0
V_3	0	0	0	$\frac{2}{\beta}\,V_4$
V_4	V_4	0	$-\frac{2}{\beta}\,V_4$	0

Table 4.4: Commutator $[V_i,V_j]$ table for the Lie algebra $\tilde{\mathcal{L}}_4$ spanned by V_i and V_j.

The resulting operators are given in Table 4.5, where each (i,j)-th entry indicates $Ad(\exp(\varepsilon\,V_i))\,V_j$.

Ad	V_1	V_2	V_3	V_4
V_1	V_1	V_2	V_3	$\exp(\varepsilon)\,V_4$
V_2	V_1	V_2	V_3	V_4
V_3	V_1	V_2	V_3	$\exp(-\frac{2\varepsilon}{\beta})\,V_4$
V_4	$V_1-\varepsilon\,V_4$	V_2	$V_3+\frac{2\varepsilon}{\beta}\,V_4$	V_4

Table 4.5: Adjoint representation table for (4.136). The (i,j)-th entry is $Ad(\exp(\varepsilon\,V_i))\,V_j$.

Using the same method suggested by Olver [80] we obtain the optimal system of subalgebras for the PDE (4.136). For the proof of Theorem 4.5 see Chapter 7.

Theorem 4.5 *A one-dimensional optimal system for the PDE (4.136) is given by the following vector fields*

(*i*) $V_1 + a_2\,V_2 + a_4\,V_3,\ V_1 + \dfrac{\beta}{2}\,V_3 + a_2\,V_2 + a_5\,V_4,$ *where* $a_4 \neq \dfrac{\beta}{2},\ a_2, a_5$ *arbitrary;*

(*ii*) $V_2 + a_4\,V_3,\ V_2 + a_5\,V_4$ *where* $a_4 \neq 0$ *and* a_5 *arbitrary;*

(*iii*) V_3; *and* (*iv*) V_4.

Vector field $V = V_1 + a_2\,V_2 + a_4\,V_3 + a_5\,V_4$

Our aim is to present a general similarity solution $F(x,t)$ for the PDE (4.136). For this purpose, we consider the one-dimensional subalgebra generated by the vector field
$v = V_1 + a_2\,V_2 + a_4\,V_3 + a_5\,V_4$, with $a_4 \neq \beta/2$, a_2, a_5 arbitrary. The solutions $G(x,t)$ of (4.151) are obtained by using the method of characteristics to be

$$G(x,t) = \frac{e^{-\alpha\,Q(t)}\,\varphi(s)}{\left[\left(1 - \frac{2a_4}{\beta}\right) R(t) + a_5\right]^2} \quad \text{where} \quad s \equiv x - \frac{a_2 + \frac{2\,a_4}{\alpha}}{1 - \frac{2\,a_4}{\beta}} \ln\left[\left(1 - \frac{2\,a_4}{\beta}\right) R(t) + a_5\right]$$

with $\varphi(s)$ an arbitrary function of s. On the other hand, using the same method of characteristics to solve (4.152), we obtain that the similarity solution and similarity variables are given by

$$F(x,t) = \frac{\psi(s)}{\left(1 - \frac{2a_4}{\beta}\right) R(t) + a_5} \quad \text{where} \quad s \equiv x - \frac{a_2 + \frac{2\,a_4}{\alpha}}{1 - \frac{2\,a_4}{\beta}} \ln\left[\left(1 - \frac{2\,a_4}{\beta}\right) R(t) + a_5\right]$$

with $\psi(s)$ an arbitrary function of s. Substituting F, F_t and F_x into the PDE (4.136) we obtain that (4.136) becomes an ODE for $\psi(s)$ in terms of $\varphi(s)$

$$\psi'(s) = \frac{\frac{\alpha}{2}\,\psi^2(s) + \left(1 - \frac{2a_4}{\beta}\right)\psi(s) + \varphi(s)}{\beta\,\psi(s) - \left(a_2 + \frac{2a_4}{\alpha}\right)}$$

The result obtained above can be formulated as follows

Theorem 4.6 *Assume $\varphi(s)$ is a completely monotonic function in s and $G(x,t)$ is given by*

$$G(x,t) = \frac{e^{-\alpha Q(t)}}{\left[\left(1 - \frac{2a_4}{\beta}\right) R(t) + a_5\right]^2}\, \varphi(s)$$

where s is the similarity variable given by

$$s \equiv x - \frac{a_2 + \frac{2a_4}{\alpha}}{1 - \frac{2a_4}{\beta}} \ln\left[\left(1 - \frac{2\,a_4}{\beta}\right) R(t) + a_5\right]$$

and $R(t) = \int_0^t e^{-\alpha Q(\tau)}\, d\tau$, where the function $Q(t)$ satisfies (4.12). Then the PDE (4.136) admits a similarity solution $F(x,t)$ of the form

$$F(x,t) = \frac{\psi(s)}{\left(1 - \frac{2a_4}{\beta}\right) R(t) + a_5}.$$

The constants $a_4 \neq \frac{\beta}{2}$ and a_2 are arbitrarily chosen such that the similarity profile $\psi(s)$ satisfies the ODE

$$\psi'(s) = \frac{\frac{\alpha}{2}\, \psi^2(s) + \left(1 - \frac{2a_4}{\beta}\right) \psi(s) + \varphi(s)}{\beta\, \psi(s) - \left(a_2 + \frac{2a_4}{\alpha}\right)} \tag{4.154}$$

In addition, $\psi(s)$ is a completely monotonic function such that $\psi^{(k)}(s) \to 0$, for $k = 0, 1, \ldots$, as $s \to \infty$.

Remark 4.9 *In order to solve the equation (4.154), we have considered a few examples of functions $\varphi(s)$ such that the ODE (4.154) can be solved explicitly and the solution $\psi(s)$ and the function $\varphi(s)$ satisfy the hypotheses of Theorem 4.6.*

We present below an example of such a function $\varphi(s)$ for which we determine an explicit expression for the similarity solution $F(x,t)$ for (4.136).

Example 4.11 ***(Similarity solutions for the general PDE (4.136) associated to the coagulation equation (4.2))*** *If the function $G(x,t)$ is given by*

$$G(x,t) = \frac{2pe^{-\alpha Q(t)}}{\alpha^2\, S(t)^2} \left\{ \frac{e^{\frac{\alpha}{2\beta} x}}{S(t)^{p+1}} - \alpha\,(p+1) - \sqrt{\left[\frac{e^{\frac{\alpha}{2\beta} x}}{S(t)^{p+1}} - \alpha\,(p+1)\right]^2 - \left[\alpha\,(p+1)\right]^2} \right\} \tag{4.155}$$

where $S(t) = R(t) + a_5 = \int_0^t e^{-\alpha Q(\tau)}\, d\tau + a_5$, and $p, a_5 > 0$ are some arbitrary constants.
Then the PDE (4.136) admits a similarity solution $F(x,t)$ given by

$$F(x,t) = \frac{2}{\alpha^2 S(t)} \left\{ \frac{e^{\frac{\alpha}{2\beta} x}}{S(t)^{p+1}} - \alpha\,(p+1) \right. \\ \left. - \sqrt{\left[\frac{e^{\frac{\alpha}{2\beta} x}}{S(t)^{p+1}} - \alpha\,(p+1) \right]^2 - \left[\alpha\,(p+1)\right]^2} \right\} \tag{4.156}$$

Proof. Indeed, let us consider the function $\varphi(s) = p\,\psi(s)$, with $p > 0$. Then (4.154) becomes a separable ODE in $\psi(s)$

$$\psi'(s) = \frac{\frac{\alpha}{2}\,\psi^2(s) + \left(p + 1 - \frac{2a_4}{\beta}\right)\psi(s)}{\beta\,\psi(s) - \left(a_2 + \frac{2a_4}{\alpha}\right)} \tag{4.157}$$

In the following, we choose $a_4 = 0$ such that the condition $a_4 \neq \frac{\beta}{2}$ holds. (In principle, one can choose a_4 arbitrary). Therefore, the solution $\psi(s)$ of (4.157) satisfies the algebraic equation

$$\left\{ \frac{\frac{\alpha}{2}\,\psi(s) + p + 1}{\psi(s)} \right\}^{\frac{a_2}{p+1}} \left(\frac{\alpha}{2}\,\psi(s) + p + 1\right)^{\frac{2\beta}{\alpha}} = e^s\, A, \tag{4.158}$$

where A is an arbitrary constant of integration, which depends on the initial condition $F(x,0) = h(x)$. Taking the limit of (4.158) as $s \to \infty$ and using the fact that $\frac{2\beta}{\alpha} > 0$ and $\psi(s) \to 0$, then we obtain that $a_2 > 0$ and $A > 0$ are necessary conditions for the new equality to hold. For simplicity, consider $A = 1$ (one can rescale the space variable x).

Moreover, in terms of the function $F(x,t) = \frac{\psi(s)}{S(t)}$ and using the definition of $s = x - a_2 \ln[S(t)]$ to get $e^s = e^x\,[S(t)]^{-a_2}$, equation (4.158) reads

$$\left\{ \frac{\alpha}{2}\, F(x,t)\, S(t) + p + 1 \right\}^{\mu} = \frac{F(x,t)\, e^{\frac{p+1}{a_2} x}}{S(t)^{1-a_2}} \tag{4.159}$$

where $\mu = 1 + \frac{2\beta\,(p+1)}{\alpha\, a_2}$. To obtain an explicit solution $\psi(s)$ we consider the parameter $\mu = 2$ or $a_2 = p + 1 > 1$. Substituting these values into (4.159) we obtain the expression of the similarity solution $F(x,t)$ as in (4.156). Clearly, both functions $F(x,t)$ and $G(x,t)$ are completely monotonic for all $x \geq 0$ and they vanish to zero (together with all their derivatives w.r.t x, as $x \to \infty$).

In particular, when $t = 0$ we obtain the initial condition $h(x)$. If $a_5 \neq 0$ then $h(x)$ is given by

$$h(x) = \frac{2}{\alpha^2\, a_5}\left\{\frac{e^{\frac{\alpha}{2\beta}x}}{a_5^{p+1}} - \alpha\,(p+1) - \sqrt{\left[\frac{e^{\frac{\alpha}{2\beta}x}}{a_5^{p+1}} - \alpha\,(p+1)\right]^2 - \left[\alpha\,(p+1)\right]^2}\right\}$$

To ensure complete monotonicity of $h(x)$ we need to assume that $a_5 > 0$. If $a_5 = 0$ then the initial condition is $h(x) = 0$ and thus $c_0(\lambda) = 0$, (i.e. no particles are present at $t = 0$).

In order to determine the solution $c(\lambda, t)$ completely, we need only obtain the expression of $Q(t)$ for all $t \geq 0$ and the inverse Laplace transform of $F(x,t)$. Let us determine first the expression of $Q(t)$. For this purpose, we use again (4.12). Thus, the equation (4.156) becomes

$$e^{\alpha\, Q(t)}\, Q'(t) = \frac{2}{\alpha^2\, S(t)}\left\{\frac{e^{\frac{\alpha}{2}Q(t)}}{S(t)^{p+1}} - \alpha(p+1) - \sqrt{\left(\frac{e^{\frac{\alpha}{2}Q(t)}}{S(t)^{p+1}} - \alpha(p+1)\right)^2 - [\alpha(p+1)]^2}\right\} \tag{4.160}$$

Moreover, using the definition of $R(t) = \int_0^t e^{-\alpha\, Q(\tau)}\, d\tau$ we obtain

$$S'(t) = e^{-\alpha\, Q(t)};\quad e^{\frac{\alpha}{2}Q(t)} = \frac{1}{\sqrt{S'(t)}};\quad \text{and}\quad e^{\alpha\, Q(t)}\, Q'(t) = -\frac{S''(t)}{\alpha\, S'(t)^2}.$$

Therefore (4.168) becomes an equation in $S(t)$ of the form:

$$\begin{aligned} -\frac{\alpha}{2}\,\frac{S''(t)\, S(t)}{S'(t)^2} &= \frac{1}{\sqrt{S'(t)}\, S(t)^{p+1}} - \alpha(p+1) \\ &\quad - \sqrt{\left(\frac{1}{\sqrt{S'(t)}\, S(t)^{p+1}} - \alpha(p+1)\right)^2 - [\alpha(p+1)]^2} \end{aligned} \tag{4.161}$$

For simplicity, we denote by $w(t) := \sqrt{S'(t)}\, S(t)^{p+1}$. Thus, we obtain

$$w'(t) = \frac{w(t)\, S'(t)}{S(t)}\left(\frac{S''(t)\, S(t)}{2\, S'(t)^2} + p + 1\right).$$

So, $-\frac{\alpha}{2}\frac{S''(t)\,S(t)}{S'(t)^2} = \alpha(p+1) - \alpha\frac{w'(t)}{w(t)}\frac{S(t)}{S'(t)}$ and (4.161) becomes now

$$-\alpha\, w'(t)\,\frac{S(t)}{S'(t)} = 1 - 2\,\alpha(p+1)\,w(t) - \sqrt{1 - 2\,\alpha(p+1)\,w(t)}. \tag{4.162}$$

Denote by $z(t) = 1 - 2\,\alpha(p+1)\,w(t)$ and $y(t) = \sqrt{z(t)}$. Then for all values of $t \geq 0$ such that $z(t) > 0$ or $w(t) = \sqrt{S'(t)}\,S(t)^{p+1} < \frac{1}{2\alpha(p+1)}$ the equation above becomes a separable ODE in $z(t)$

$$\frac{z'(t)}{z(t) - \sqrt{z(t)}} = 2(p+1)\frac{S'(t)}{S(t)} \quad \Rightarrow \quad \int \frac{y}{y^2 - y}\,dy = \ln[S(t)^{p+1}].$$

Thus $C + \ln\left|\sqrt{z} - 1\right| = \ln[S(t)]^{p+1}$, where C is an integration constant. Moreover, since $w(t) > 0$ then $1 > z(t) = 1 - 2\,\alpha(p+1)\,w(t)$. Thus, we obtain

$$C\left[1 - \sqrt{1 - 2\alpha(p+1)\,w(t)}\right] = S(t)^{p+1}$$

So,

$$1 - \sqrt{1 - 2\alpha(p+1)\,\sqrt{S'(t)}\,S(t)^{p+1}} = S(t)^{p+1}\,A,$$

where $A = 1/C > 0$ (this holds since LHS above is > 0 and also $S(t)^{p+1} > 0$). The equation above can be rewritten in the following form

$$\sqrt{S'(t)} = \frac{1}{2\alpha(p+1)}\left(2\,A - A^2\,S(t)^{p+1}\right).$$

Since $S(0) = R(0) + a_5 = a_5$ (as $R(0) = 0$) and $S'(0) = R'(0) = 1$ then if we set $t = 0$ we obtain that the constant A is given by the equation $A^2\,a_5^{p+1} - 2\,A + 2\alpha(p+1) = 0$. If $a_5 = 0$ then we get $A = \alpha(p+1)$, and if $a_5 \neq 0$ we can rescale the time variable such that $a_5 = 1$ and in this case we obtain $A = 1 - \sqrt{1 - 2\alpha(p+1)} > 0$, and we need to assume that $\alpha \in (0, \frac{1}{2})$ and $p \in (0, \frac{1}{2\alpha} - 1]$. Therefore, in this case, we obtain

$$S(t)^{p+1} = \frac{2}{A}\left\{1 - \frac{\alpha(p+1)}{A}\,\sqrt{S'(t)}\right\}$$

Taking the derivative w.r.t. t on both sides and using the definition of $S(t)$ we obtain

$$\frac{\alpha}{2}\,e^{\frac{\alpha}{2}Q(t)}\,Q'(t) = \frac{A}{\alpha}\left(\frac{A}{2}\right)^{\frac{1}{p+1}}\left\{1 - \frac{\alpha(p+1)}{A}\,e^{-\frac{\alpha}{2}Q(t)}\right\}^{\frac{p}{p+1}}$$

If we denote by $v(t) := e^{\frac{\alpha}{2}Q(t)}$ then we obtain an I.V.P for $v(t)$ (where we make use of $Q(0) = 0$):

$$v'(t) = \frac{A}{\alpha}\left(\frac{A}{2}\right)^{\frac{1}{p+1}}\frac{\left(v(t) - \frac{\alpha(p+1)}{A}\right)^{\frac{p}{p+1}}}{v(t)^{\frac{p}{p+1}}} \quad \text{subject to I.C} \quad v(0) = 1. \tag{4.163}$$

This equation is valid only for values of t such that $t \in [0, T_c)$, where T_c is obtained as an upper bound (if any) of the solution to the inequality $w(t) < \frac{1}{2\alpha(p+1)}$. The last inequality is equivalent to $v(t) < \frac{2\alpha(p+1)}{A}$ and using (4.163), one can prove that there is a time T_c such that $v(T_c) = \frac{2\alpha(p+1)}{A}$. One can solve the equation (4.163) and determine an implicit formula for $v(t) = e^{\frac{\alpha}{2} Q(t)}$ and thus obtain

$$S(t) = \int_0^t e^{-\alpha Q(\tau)}\, d\tau + a_5 \quad \text{for all values } t \in [0, T_c).$$

In general, numerical methods need to be employed in order to solve (4.163). We leave this for future work.

On the other hand for values of t such that $w(t) = \sqrt{S'(t)}\, S(t)^{p+1} \geq \frac{1}{2\alpha(p+1)}$, the equation (4.162) has the solution $w(t) = \frac{1}{2\alpha(p+1)}$. Thus, $S(t)$ satisfies the I.V.P.

$$\sqrt{S'(t)}\, S(t)^{p+1} = \frac{1}{2\alpha(p+1)} \qquad \text{subject to I.C.} \quad S(T_c) = \lim_{t \to T_c} S(t) \tag{4.164}$$

where, in the last equality $S(t)$ is given by (4.163). Next, we solve (4.164) by simply integrating it w.r.t t from T_c to t and obtain

$$S(t)^{2p+3} = S(T_c)^{2p+3} + \frac{2p+3}{4\,\alpha^2\,(p+1)^2}\,(t - T_c) \quad \text{for } t \geq T_c. \tag{4.165}$$

Conjecture 4.1 *Similar to 4.2.3, one can prove that the time T_c above corresponds in fact to the gelation time T_{gel}. However, we leave the proof of this statement for future work.*

In particular, if $p = 1$ then we can solve the ODE (4.163) and obtain that $v(t)$ is given implicitly by the equation

$$\sqrt{v(t)\,(v(t) - q)} + q \ln\left(\frac{v(t) + \sqrt{v(t) - q}}{1 + \sqrt{1 - q}}\right) = \frac{A}{\alpha}\left(\frac{A}{2}\right)^{1/2} t + \sqrt{1 - q} \tag{4.166}$$

where $q = \frac{2\alpha}{A}$. Therefore, in this case we obtain an implicit equation for $Q(t)$

$$\sqrt{e^{\frac{\alpha}{2} Q(t)}\,(e^{\frac{\alpha}{2} Q(t)} - q)} + q \ln\left(\frac{e^{\frac{\alpha}{2} Q(t)} + \sqrt{e^{\frac{\alpha}{2} Q(t)} - q}}{1 + \sqrt{1 - q}}\right) = \frac{A}{\alpha}\left(\frac{A}{2}\right)^{1/2} t + \sqrt{1 - q}. \tag{4.167}$$

This equation is valid for values $t \in [0, T_c)$, where T_c is an upper bound of the inequality $\sqrt{S'(t)}\, S(t)^2 < \frac{1}{4\alpha}$, where $S(t) = \int_0^t e^{-\alpha Q(\tau)}\, d\tau + a_5$, where $a_5 \geq 0$. Next, using $Q(t)$ from the equation (4.167), one obtains $S(T_c) = \lim_{t \to T_c} S(t)$ and use this as an I.C. to solve the I.V.P (4.164). Using (4.167) and $v(T_c) = \frac{2\alpha(p+1)}{A}$, we determine T_c in the particular case $p = 1$ to be

$$T_c = \frac{\alpha}{A} \sqrt{\frac{2}{A}} \left(q\sqrt{2} + q \ln\left(\frac{2q + \sqrt{q}}{1 + \sqrt{1-q}} \right) - \sqrt{1-q} \right)$$

Using a similar approach as in 4.2.4 we determine the behaviour of the solution $c(\lambda, t)$ of (4.2) for $\lambda \to \infty$ and all $t \geq 0$. In addition, we also present a series solution for $c(\lambda, t)$.

Asymptotic and formal series solution

The function $F(x, t)$ in (4.156) has a branch point $x_0 = x_0(t) = \frac{2\beta}{\alpha} \ln\Big[2\alpha(p + 1) S(t)^{p+1}\Big]$.
Expanding $F(x, t)$ about the branch point $x_0(t)$ we obtain

$$F(x,t) \sim \frac{2(p+1)}{\alpha S(t)} - \frac{4(p+1)\sqrt{\frac{\alpha}{2\beta}}}{\alpha S(t)} \big(x - x_0(t)\big)^{1/2} + \mathcal{O}\big(x - x_0(t)\big) \quad \text{as} \quad x \to x_0(t).$$

Therefore, according to [23] we obtain the asymptotic behaviour of the solution $f(\lambda, t)$ as $\lambda \to \infty$ to be

$$(\alpha + \beta\lambda)\, f(\lambda, t) \sim \frac{(p+1)\, \lambda^{-3/2}}{\alpha\, S(t)} \sqrt{\frac{2\,\alpha}{\beta\pi}} \Big[2\alpha(p+1)\, S(t)^{p+1}\Big]^{\frac{2\beta}{\alpha}\lambda}.$$

Using the definition of $c(\lambda, t)$ we obtain the asymptotic behaviour for the solution $c(\lambda, t)$ of (4.2) as $\lambda \to \infty$ for all $t \geq 0$ to be

$$c(\lambda, t) \sim \frac{\lambda^{-3/2}\, e^{-(\alpha+\beta\lambda)\, Q(t)}}{(\alpha + \beta\lambda)\, \alpha\, S(t)} \sqrt{\frac{2\,\alpha}{\beta\pi}} \Big[2\alpha(p+1) S(t)^{p+1}\Big]^{\frac{2\beta}{\alpha}\lambda} \quad \text{as} \quad \lambda \to \infty, \quad \forall t \geq 0$$

Moreover, we can also obtain the solution $c(\lambda, t)$ to (4.2) in series form. For this purpose, we expand the square root in $F(x, t)$ defined by (4.156) using the binomial theorem

$$
\begin{aligned}
F(x,t) &= \frac{2}{\alpha^2\,S(t)}\left\{\frac{e^{\frac{\alpha}{2\beta}x}}{S(t)^{p+1}} - \alpha\,(p+1) - \frac{e^{\frac{\alpha}{2\beta}x}}{S(t)^{p+1}}\left(1 - \frac{2\,\alpha(p+1)S(t)^{p+1}}{e^{\frac{\alpha}{2\beta}x}}\right)^{1/2}\right\} \\
&= \frac{2}{\alpha^2\,S(t)}\left\{\frac{e^{\frac{\alpha}{2\beta}x}}{S(t)^{p+1}} - \alpha\,(p+1) - \frac{e^{\frac{\alpha}{2\beta}x}}{S(t)^{p+1}}\sum_{k=0}^{\infty}(-1)^k\binom{1/2}{k}\left(\frac{2\alpha(p+1)S(t)^{p+1}}{e^{\frac{\alpha}{2\beta}x}}\right)^k\right\} \\
&= \frac{2}{\alpha^2\,S(t)}\sum_{k=2}^{\infty}(-1)^{k+1}\binom{1/2}{k}\left[2\alpha(p+1)S(t)^{p+1}\right]^k e^{-\frac{\alpha\,(k-1)}{2\beta}x} \qquad (4.168)
\end{aligned}
$$

Next, we formally take the inverse Laplace transform term by term to get the inverse Laplace transform of $F(x,t)$ Thus we obtain the solution $c(\lambda,t)$ of the coagulation equation becomes

$$
c(\lambda,t) = \frac{2\,e^{-(\alpha+\beta\lambda)\,Q(t)}}{(\alpha+\beta\lambda)\,\alpha^2\,S(t)}\sum_{k=2}^{\infty}\frac{(2k-2)!}{2^{2k-1}k!(k-1)!}\left[2\alpha(p+1)S(t)^{p+1}\right]^k\,\delta\Big(\lambda - \frac{\alpha\,(k-1)}{2\beta}\Big)
$$

where $S(t)$ is determined above and the initial condition is given by:

(a) If $a_5 \neq 0$ then

$$
c_0(\lambda) = \frac{2}{(\alpha+\beta\lambda)\,\alpha^2\,a_5}\sum_{k=2}^{\infty}\frac{(2k-2)!}{2^{2k-1}k!(k-1)!}\left[2\alpha(p+1)\,a_5^{p+1}\right]^k\,\delta\Big(\lambda - \frac{\alpha\,(k-1)}{2\beta}\Big)
$$

(b) If $a_5 = 0$ then $c_0(\lambda) = 0$ which corresponds to the case when no particles are initially present in the system.

4.3 Symmetry methods applied directly to the coagulation equation

We apply a new generalized version of the direct methods that determine the symmetry group of point transformations for integro-differential equations to the coagulation equation in the presence of source terms. These methods provide us with a new family of similarity solutions to the coagulation equations which can be further used for numerical studies. Due to the presence of the non-local (integral) terms, the classical approaches for investigating the symmetry groups of differential equations cannot be applied directly to integro-differential equations (IDEs).

The existence of symmetry groups for IDEs with non-local structure has been developed only recently in the work of Zawistowski [112], Akhiev et al. [4]. Applications of this method are currently provided for a few classes of IDEs, such as: Vlasov-Maxwell equations, collisionless-Boltzmann equations and fragmentation equation [32]. Some very special cases of IDEs can be reduced to differential equations. However, this is not the case of the most important IDEs in physics such as equations of kinetic theory. Coagulation equations are such examples of equations that cannot always be reduced to PDEs, if for example the coagulation kernel is not a bilinear, separable kernel (see Section 4.2) or has coefficients that depend on time t, as is the case in this section.

The study related to the symmetry groups for coagulation equations has not received much attention in the literature. The main difficulty for developing a direct and general theory is related to the existence of the integral terms in these equations, in particular the convolution-type integral with nonlinear functions. In the literature of coagulation equations, Chetverikov and Kudryavtsev [20] are the first to construct a theory of symmetries and conservation laws for IDEs. The authors provide a method that is known as the method of boundary differential equations, which is applied to the coagulation kinetic equation by reducing this equation into a boundary differential equation and using the concept of covering (see e.g. [20]).

In this section, we provide a more general and direct method for determining a point symmetry group for coagulation equations with particle source terms. In our study, we extend the direct methods proposed by Akhiev et al. [4] that determine the symmetry group of point transformations to IDEs. We propose a new generalized method for dealing with the convolution-type integral by transforming the coagulation equation into a system that consists of an IDE and a PDE. For this purpose, we make use of the general definition of the point symmetry group for IDEs and the extended infinitesimal generator that includes the nonlocal variables as the variables of the jet space as given in the recent work of Zawistowski [112] and later by Akhiev et al. [4]. We obtain some similarity solutions and similarity reductions of the coagulation equation for the case when the kernel function K is a bilinear, separable function that may depend on the time variable t. For some particular kernels we have also obtained the expressions of the total mass, and studied the occurrence of the gelation phenomena. The group method is applied to a modified coagulation equation (4.176) that involves only the convolution integral. To our knowledge, this is the first example of application of the symmetry group to convolution-type integro-differential equations. The method that we propose in this section can be extended to include other special cases of coagulation kernels, and nonlocal terms.

The advantage of this method over the previous methods used in the self-similarity theory is that we obtain a few similarity solutions without assuming a priori any special ansatz or structure of the scaling solutions to the coagulation equation as assumed in the work of [35, 36, 45, 24].

4.3.1 New modified version of the coagulation equation

Consider the coagulation equation with particle source terms given by

$$\frac{\partial c}{\partial t}(\lambda,t) = \frac{1}{2}\int_0^\lambda K(\lambda-\mu,\mu,t)c(\lambda-\mu,t)c(\mu,t)d\mu - c(\lambda,t)\int_0^\infty K(\lambda,\mu,t)c(\mu,t)d\mu + g(\lambda,t) \tag{4.169}$$

subject to the initial condition

$$c(\lambda,0) = c_0(\lambda), \tag{4.170}$$

where the space variable λ and the time variable t range in the interval $[0,\infty)$.

In this section, we assume that the rate of coagulation of particles or the kernel $K(\lambda,\mu,t)$ and the source function $g(\lambda,t)$ are both non-negative functions. In addition, we assume the coagulation kernel is a separable and bilinear function whose coefficients depend on time t

$$K(\lambda,\mu,t) = \theta(\lambda,t)\,\theta(\mu,t), \quad \text{where} \quad \theta(\lambda,t) = \alpha(t) + \beta(t)\lambda \tag{4.171}$$

for any λ, $t \geq 0$, where $\alpha(t)$ and $\beta(t)$ are arbitrary non-negative functions of t.

For the moment, the functions $\alpha(t)$ and $\beta(t)$ are assumed to be arbitrary. Specific examples of such functions and special examples of source terms will be established later in this section in such a way that similarity solutions for the coagulation equation (4.169) exist. As part of our analysis, we allow the coagulation kernel to have one of the following forms:

(a) $K(\lambda,\mu,t) = \alpha^2(t)$;

(b) $K(\lambda,\mu,t) = \beta^2(t)\,\lambda\,\mu$;

(c) $K(\lambda,\mu,t) = (\alpha_0 + \beta_0\,\lambda)\,(\alpha_0 + \beta_0\,\mu)$, where α_0, $\beta_0 > 0$ are some arbitrary constants,

and $\alpha(t)$ and $\beta(t)$ arbitrary at this point. However, we will show in this section that these functions satisfy a coupled system of ODEs.

Due to the very special form (4.171) of the coagulation kernel K we make the following notation

$$N(t) = \int_0^\infty \theta(\lambda,t)\,c(\lambda,t)\,d\lambda = \alpha(t)\,M_0(t) + \beta(t)\,M_1(t),$$

where $M_0(t)$ and $M_1(t)$ represent the zeroth and first moments of the solution $c(\lambda,t)$, respectively as defined in (4.5). Using the above notations, equation (4.169) becomes:

$$\frac{\partial c}{\partial t}(\lambda,t) + \theta(\lambda,t)\,N(t)\,c(\lambda,t) = \frac{1}{2}\int_0^\lambda \theta(\lambda-\mu,t)\,\theta(\mu,t)c(\lambda-\mu,t)c(\mu,t)\,d\mu \;+\; g(\lambda,t) \tag{4.172}$$

We begin by eliminating the "infinite integral" from the equation (4.172), in the form of the function $\theta(\lambda,t)\,N(t)\,c(\lambda,t)$ by means of an integrating factor. For this reason, let

$$\Phi(\lambda,t) := \int_0^t \theta(\lambda,\tau)N(\tau)d\tau = \int_0^t (\alpha(\tau) + \lambda\beta(\tau))N(\tau)d\tau \text{ and} \tag{4.173}$$

$$Y(t) := \int_0^t \alpha(\tau)N(\tau)d\tau. \tag{4.174}$$

We multiply the equation (4.172) by $e^{\Phi(\lambda,t)}\,e^{(\alpha_0+\beta_0\,\lambda)\,\sigma} = e^{\Phi(\lambda,t)}\,e^{\theta(\lambda,0)\,\sigma}$, where $\alpha_0 = \alpha(0)$, $\beta_0 = \beta(0)$, and σ are arbitrary real numbers. The parameter σ has been included here for physical reasons, as will be explained later in this section. Using the above notations we rewrite the convolution integral in (4.172) in the following form

$$e^{-(Y(t)+\alpha_0\sigma)} \int_0^{\lambda} \theta(\lambda-\mu,t)\theta(\mu,t) \left\{ e^{\Phi(\lambda-\mu,t)} e^{\theta(\lambda-\mu,0)\sigma} c(\lambda-\mu,t) \right\} \left\{ e^{\Phi(\mu,t)} e^{\theta(\mu,0)\sigma} c(\mu,t) \right\} d\mu$$

Moreover, for simplicity we define the functions

$$f(\lambda,t) = c(\lambda,t)\, e^{\Phi(\lambda,t)}\, e^{\theta(\lambda,0)\,\sigma} \quad \text{and} \quad h(\lambda,t) = g(\lambda,t)\, e^{\Phi(\lambda,t)}\, e^{\theta(\lambda,0)\,\sigma} \tag{4.175}$$

Thus, we obtain a new modified version of the coagulation equation (4.169):

$$\frac{\partial f}{\partial t}(\lambda,t) = \frac{1}{2}\, e^{-(Y(t)+\alpha_0\sigma)} \int_0^{\lambda} \theta(\lambda-\mu,t)\, \theta(\mu,t)\, f(\lambda-\mu,t)\, f(\mu,t)\, d\mu \,+\, h(\lambda,t) \tag{4.176}$$

subject to the initial condition

$$f(\lambda,0) = f_0(\lambda) = e^{(\alpha_0+\beta_0\,\lambda)\,\sigma}\, c_0(\lambda) \tag{4.177}$$

where f and h represent the new solution and source term of the modified coagulation equation (4.176).

Since the group symmetry method is independent of the initial condition, we disregard for the moment the initial condition (4.177) and concentrate only on the new form of the coagulation equation (4.176). We will take the initial condition into account when we have determined the form of the similarity solution $f(\lambda,t)$ with the purpose of providing explicit (analytic) or asymptotic large size ($\lambda \to \infty$) behaviour of solutions f and thus c.

4.3.2 Transformation of the coagulation equation into a system of PIDEs

In order to illustrate our method we make some transformations to the equation (4.176). First, we rewrite (4.176) such that the limits of integration are independent of λ. This can be achieved with the help of the Heaviside step unit function

$$H(\lambda) = \begin{cases} 1, & \text{if } \lambda > 0 \\ 0, & \text{if } \lambda < 0 \end{cases}$$

Therefore, the convolution integral in (4.176) takes the form

$$\int_0^\infty P(\lambda,\mu)\,\theta(\lambda-\mu,t)\,\theta(\mu,t)\,f(\lambda-\mu,t)\,f(\mu,t)\,d\mu$$

where $P(\lambda,\mu) = 1 - H(\mu-\lambda)$. Next, let

$$v(\lambda,\mu,t) = P(\lambda,\mu)\,\theta(\lambda-\mu,t)\,f(\lambda-\mu,t)$$

If we calculate the partial derivatives of v, then we obtain the following PDE for the function $v(\lambda,\mu,t)$

$$v_\lambda + v_\mu = 0.$$

Using the transformations above, the coagulation equation (4.176) changes into a coupled system of IDE and PDE in f and v, or a system of partial integro-differential equations (PIDEs) of the form

$$\begin{aligned}
&\frac{\partial f}{\partial t}(\lambda,t) = \frac{1}{2}\,e^{-(\Upsilon(t)+\alpha_0\,\sigma)} \int_0^\infty v(\lambda,\mu,t)\,f(\mu,t)\,\theta(\mu,t)\,d\mu + h(\lambda,t)\\
&v_\lambda + v_\mu = 0
\end{aligned} \tag{4.178}$$

4.3.3 Symmetry groups of point transformations for the coagulation equation. Theoretical approach

In this subsection we adapt the theoretical description in Section 3.2 for a general first order PDE and apply this to the system (4.178) in order to determine a Lie symmetry group of point transformations (see e.g. the articles [4, 112] for the collisionless Boltzmann equation). For the new system (4.178), we need to impose the invariance conditions to both the IDE and the PDE, and solve a system of determining equations, that consists of both local (PDEs) and nonlocal equations (IDEs). These new determining equations that we derive are much easier to solve than the original coagulation equation. We present a new approach for solving the resulting system of determining equations which, to our knowledge, are new to the theory of coagulation equations. The approach we suggest below can be applied to other special cases of integro-differential equations of the form (4.176) or (4.169).

First, we consider the equations in the system (4.178) as two surfaces $\mathcal{F}_1$ and $\mathcal{F}_2$ defined by

$$\begin{aligned} \mathcal{F}_1 &\equiv f_t - \frac{1}{2}\, e^{-(Y(t)+\alpha_0\,\sigma)}\, T(f,v) - h(\lambda,t) = 0 \\ \mathcal{F}_2 &\equiv v_\lambda + v_\mu = 0 \end{aligned} \tag{4.179}$$

given in the space of variables $(t,\, \lambda,\, \mu,\, f,\, f_t,\, v_\lambda,\, v_\mu,\, T(f,v))$, where

$$T(f,v) = \int_0^\infty f\, v\, \theta(\mu,t)\, d\mu = \int_0^\infty m(\mu,\, v,\, f,\, t)\, d\mu$$

represents the nonlocal variable (integro-differential operator), where for simplicity we let

$$m(\mu,\, v,\, f,\, t) = f\, v\, \theta(\mu,t) = \big(\alpha(t) + \beta(t)\mu\big)\, f\, v.$$

As described in Section 3.2, we look for a Lie group of point transformations admitted by the PIDE system (4.178). For this purpose, we concentrate now on the system of equations above which we write in the following general form

$$\begin{aligned} &\mathcal{F}_1(\lambda,\, \mu,\, t,\, f(\lambda,t),\, f_t(\lambda,t),\, v(\lambda,\, \mu,\, t),\, T(f,v)(\lambda,t)) = 0 \\ &\mathcal{F}_2(\lambda,\, \mu,\, t,\, v(\lambda,\mu,t),\, v_\lambda(\lambda,\mu,t),\, v_\mu(\lambda,\mu,t)) = 0. \end{aligned} \tag{4.180}$$

Next, we consider the one-parameter (ε) Lie group of point transformations:

$$\begin{aligned} \tilde{\lambda} &= e^{\varepsilon G}(\lambda) = \lambda + \varepsilon\, \xi_1(\lambda,\, \mu,\, t,\, f,\, v) + O(\varepsilon^2) \\ \tilde{\mu} &= e^{\varepsilon G}(\mu) = \mu + \varepsilon\, \xi_2(\lambda,\, \mu,\, t,\, f,\, v) + O(\varepsilon^2) \\ \tilde{t} &= e^{\varepsilon G}(t) = t + \varepsilon\, \xi_3(\lambda,\, \mu,\, t,\, f,\, v) + O(\varepsilon^2) \\ \tilde{f} &= e^{\varepsilon G}(f) = f + \varepsilon\, \eta_1(\lambda,\, \mu,\, t,\, f,\, v) + O(\varepsilon^2) \\ \tilde{v} &= e^{\varepsilon G}(v) = v + \varepsilon\, \eta_2(\lambda,\, \mu,\, t,\, f,\, v) + O(\varepsilon^2) \end{aligned} \tag{4.181}$$

with the infinitesimal generator

$$G = \xi_1 \frac{\partial}{\partial \lambda} + \xi_2 \frac{\partial}{\partial \mu} + \xi_3 \frac{\partial}{\partial t} + \eta_1 \frac{\partial}{\partial f} + \eta_2 \frac{\partial}{\partial v}$$

where $\xi_j(\lambda,\, \mu,\, t,\, f,\, v)$ and $\eta_i(\lambda,\, \mu,\, t,\, f,\, v)$ are sufficiently smooth functions, which represent the generators of the point group of transformations.

Similar to the Ovsiannikov's method for DEs [81] and following the theoretical description in Section 3.2 for PDEs, we consider the 1^{st} order extension of the group

(4.181) from the space of variables (λ, μ, t, f, v) into the space of independent and dependent variables, and derivatives of dependent variables $(\lambda, \mu, t, f, v, f_t, v_\lambda, v_\mu)$

$$\begin{aligned}
\tilde{\lambda} &= e^{\varepsilon G^{(1)}}(\lambda) = \lambda + \varepsilon\, \xi_1(\lambda,\, \mu,\, t,\, f,\, v) + O(\varepsilon^2) \\
\tilde{\mu} &= e^{\varepsilon G^{(1)}}(\mu) = \mu + \varepsilon\, \xi_2(\lambda,\, \mu,\, t,\, f,\, v) + O(\varepsilon^2) \\
\tilde{t} &= e^{\varepsilon G^{(1)}}(t) = t + \varepsilon\, \xi_3(\lambda,\, \mu,\, t,\, f,\, v) + O(\varepsilon^2) \\
\tilde{f} &= e^{\varepsilon G^{(1)}}(f) = f + \varepsilon\, \eta_1(\lambda,\, \mu,\, t,\, f,\, v) + O(\varepsilon^2) \\
\tilde{v} &= e^{\varepsilon G^{(1)}}(v) = v + \varepsilon\, \eta_2(\lambda,\, \mu,\, t,\, f,\, v) + O(\varepsilon^2) \\
\tilde{f}_{\tilde{t}} &= e^{\varepsilon G^{(1)}}(f_t) = f_t + \varepsilon\, \eta_1^t + O(\varepsilon^2) \\
\tilde{v}_{\tilde{\lambda}} &= e^{\varepsilon G^{(1)}}(v_\lambda) = v_\lambda + \varepsilon\, \eta_2^\lambda + O(\varepsilon^2) \\
\tilde{v}_{\tilde{\mu}} &= e^{\varepsilon G^{(1)}}(v_\mu) = v_\mu + \varepsilon\, \eta_2^\mu + O(\varepsilon^2)
\end{aligned} \tag{4.182}$$

where η_1^t, η_2^λ, η_2^μ represent the infinitesimals of the group defined by (see e.g. [4])

$$\begin{aligned}
\eta_1^t &= \eta_{1,t} + (\eta_{1,f} - \xi_{3,t})\, f_t - \xi_{1,t}\, f_\lambda - \xi_{3,f}\, f_t^2 - \xi_{1,f}\, f_\lambda\, f_t \\
\eta_2^\lambda &= \eta_{2,\lambda} + (\eta_{2,v} - \xi_{1,\lambda})\, v_\lambda - \xi_{3,\lambda}\, v_t - \xi_{1,v}\, v_\lambda^2 - \xi_{3,v}\, v_\lambda\, v_t \\
\eta_2^\mu &= \eta_{2,\mu} + (\eta_{2,v} - \xi_{1,\mu})\, v_\mu - \xi_{3,\mu}\, v_t - \xi_{1,v}\, v_\mu^2 - \xi_{3,v}\, v_\mu\, v_t
\end{aligned}$$

and $G^{(1)}$ represents the extended infinitesimal generator given by

$$G^{(1)} = G + \eta_1^t \frac{\partial}{\partial f_t} + \eta_2^\lambda \frac{\partial}{\partial v_\lambda} + \eta_2^\mu \frac{\partial}{\partial v_\mu}.$$

Similar as in Section 3.2, invariance of a system of equations means invariance of the space of its solutions. Therefore, the point transformation (4.182) maps any solution $\{f, v\}$ of the system of PIDE (4.179) into another solution $\{\tilde{f}, \tilde{v}\}$ of the same system of equations. In our geometric language, where solutions are represented by their graphs in a jet space, the above can be formulated as follows

Definition 6 ***(Criterion of invariance of the system of PIDEs (4.180))*** *If the system of PIDEs (4.180) transforms to the following form of invariant equations under the group of point transformations (4.182) then this group is called a point symmetry group for the system of equations:*

$$\begin{aligned}
&\mathcal{F}_1(\tilde{\lambda},\, \tilde{\mu},\, \tilde{t},\, \tilde{f}(\tilde{\lambda}, \tilde{t}),\, \tilde{f}_{\tilde{t}}(\tilde{\lambda}, \tilde{t}),\, \tilde{v}(\tilde{\lambda},\, \tilde{\mu},\, \tilde{t}),\, \tilde{T}(\tilde{f}, \tilde{v})(\tilde{\lambda}, \tilde{t})) = 0 \\
&\mathcal{F}_2(\tilde{\lambda},\, \tilde{\mu},\, \tilde{t},\, \tilde{v}(\tilde{\lambda}, \tilde{\mu}, \tilde{t}),\, \tilde{v}_{\tilde{\lambda}}(\tilde{\lambda}, \tilde{\mu}, \tilde{t}),\, \tilde{v}_{\tilde{\mu}}(\tilde{\lambda}, \tilde{\mu}, \tilde{t})) = 0
\end{aligned} \tag{4.183}$$

where

$$\tilde{T}(\tilde{f},\tilde{v})(\tilde{\lambda},\tilde{t}) = \int_0^{\infty} m(\tilde{\mu},\tilde{f},\tilde{v},\tilde{t})\, d\tilde{\mu} \tag{4.184}$$

is obtained by the extended transformation (4.182).

According to (4.184), we act on the system of PIDEs (4.180) by extended transformations (4.182) writing down explicitly only terms up to the order ε, that is linear terms with respect to the parameter ε. Next, we expand in Taylor series the integrand function m in (4.184). After changing the integral variable and applying (4.182) we obtain that the nonlocal term $\tilde{T}(\tilde{f},\tilde{v})(\tilde{\lambda},\tilde{t})$ has the form

$$\tilde{T}(\tilde{f},\tilde{v}) = T(f,v) + \varepsilon\, P_T(f,v) + O(\varepsilon^2) \tag{4.185}$$

where P_T is given by

$$\begin{aligned} P_T(f,v) = \int_0^{\infty} \Big\{ & \xi_1 \frac{\partial m}{\partial \lambda} + \xi_2 \frac{\partial m}{\partial \mu} + \xi_3 \frac{\partial m}{\partial t} + \eta_1 \frac{\partial m}{\partial f} + \eta_2 \frac{\partial m}{\partial v} \\ & + m \left(\frac{\partial \xi_2}{\partial \mu} + \frac{\partial \xi_2}{\partial f}\frac{\partial f}{\partial \mu} + \frac{\partial \xi_2}{\partial v}\frac{\partial v}{\partial \mu} \right) \Big\}\, d\mu \end{aligned} \tag{4.186}$$

Consequently, the extension of the point group (4.182) on the nonlocal variable $T(f,v)$ is defined by (4.182, 4.185). Therefore, we can consider the generator of the extended group (4.182, 4.185) as follows

$$G_T^{(1)} = G^{(1)} + P_T(f,v)\, \frac{\partial}{\partial(T(f,v))}. \tag{4.187}$$

Substituting the expressions (4.182), (4.185), (4.186) and (4.187) into the general system (4.183), and using Taylor expansion, the invariance criterion of the system of PIDEs (4.180) under the group of transformations gives the following

Definition 7 ***(Determining equations for the system of PIDE (4.180))*** *The PIDE system (4.183) is said to be invariant under the point group of transformations (4.182, 4.185) if and only if the following system of determining equations holds*

$$G_T^{(1)}\, \mathcal{F}_1(\lambda,\mu,t,f,f_t,v,T(f,v)) = 0 \tag{4.188}$$

$$G_T^{(1)}\, \mathcal{F}_2(\lambda,\mu,t,v,v_\lambda,v_\mu) = 0 \tag{4.189}$$

for any arbitrary solutions $f(\lambda, t)$ and $v(\lambda, \mu, t)$ of the system (4.183) of PIDEs. The infinitesimal generator of the extended group (4.182, 4.185) is defined by the operator

$$G_T^{(1)} = \xi_1 \frac{\partial}{\partial \lambda} + \xi_2 \frac{\partial}{\partial \mu} + \xi_3 \frac{\partial}{\partial t} + \eta_1 \frac{\partial}{\partial f} + \eta_2 \frac{\partial}{\partial v} + \eta_1^t \frac{\partial}{\partial f_t} + P_T(f,v) \frac{\partial}{\partial (T(f,v))} + \eta_2^\lambda \frac{\partial}{\partial v_\lambda} + \eta_2^\mu \frac{\partial}{\partial v_\mu} \tag{4.190}$$

In the following, we apply the theoretical approach presented above to the system (4.179) of PIDEs. In particular, we apply the extended generator $G_T^{(1)}$ defined by (4.190) to the frames (surfaces) $\mathcal{F}_1$ and $\mathcal{F}_2$ to obtain the invariance criteria for (4.179). The solutions of the determining equations will provide us with similarity solutions to the modified and original coagulation equation, respectively. For some initial conditions these solutions are in fact analytical solutions, while in other cases they are only similarity solutions or group invariant solutions, nevertheless any type of solution that we obtain is of interest for our study.

4.3.4 Determining equations for the system of PIDEs

The invariance condition for Eq. $\mathcal{F}_1 = 0$

Using (4.190), the definition (4.179) of $\mathcal{F}_1$ and η_1^t, the determining equation (4.188) takes the form

$$\begin{aligned} -\xi_1 \frac{\partial h}{\partial \lambda} + \xi_3 \left[\frac{1}{2} e^{-(Y(t)+\alpha_0 \sigma)} Y'(t)\, T(f,v) - \frac{\partial h}{\partial t}\right] + \frac{\partial \eta_1}{\partial t} - \frac{\partial \xi_1}{\partial t} f_\lambda - \frac{\partial \xi_3}{\partial f} f_t^2 - \frac{\partial \xi_1}{\partial f} f_\lambda f_t \\ + \left(\frac{\partial \eta_1}{\partial f} - \frac{\partial \xi_3}{\partial t}\right)\left(\frac{1}{2} e^{-(Y(t)+\alpha_0 \sigma)} T(f,v) + h(\lambda,t)\right) - \frac{1}{2} P_T(f,v)\, e^{-(Y(t)+\alpha_0 \sigma)} = 0 \end{aligned} \tag{4.191}$$

where

$$\begin{aligned} P_T(f,v) = \int_0^\infty \Bigg\{ \left[\xi_2\, \beta(t) + \xi_3 \frac{\partial \theta}{\partial t}(\mu,t)\right] f\, v + \eta_1\, v\, \theta(\mu,t) + \eta_2\, f\, \theta(\mu,t) + \theta(\mu,t)\, f\, v \frac{\partial \xi_2}{\partial \mu} \\ + f\, v\, \theta(\mu,t) \frac{\partial \xi_2}{\partial f} f_\mu + f\, v\, \theta(\mu,t) \frac{\partial \xi_2}{\partial v} v_\mu \Bigg\}\, d\mu \end{aligned} \tag{4.192}$$

Since the left hand-side of (4.191) is a sum of local and nonlocal terms, we split (4.191) into local terms **(LT)** and nonlocal terms **(NLT)**. Thus we obtain

The local term of (4.191) is given by

$$\mathbf{LT}:\ -\xi_1\frac{\partial h}{\partial \lambda}-\xi_3\frac{\partial h}{\partial t}+\frac{\partial \eta_1}{\partial t}+\Big(\frac{\partial \eta_1}{\partial f}-\frac{\partial \xi_3}{\partial t}\Big)h(\lambda,t)-\frac{\partial \xi_1}{\partial t}f_\lambda-\frac{\partial \xi_3}{\partial f}f_t^2-\frac{\partial \xi_1}{\partial f}f_\lambda\,f_t=0 \tag{4.193}$$

To solve (4.193), we use the standard Lie algorithm as in Section 4.2. This reduces to splitting **LT** with respect to the local variables and their derivatives, and equating like derivatives to zero (see e.g. [4, 12]). Thus, setting the coefficients of like derivatives to zero, we obtain

$$f_\lambda \text{ terms}: \quad \xi_{1,t}=0 \tag{4.194}$$

$$f_\lambda\, f_t \text{ terms}: \quad \xi_{1,f}=0 \tag{4.195}$$

$$f_t^2 \text{ terms}: \quad \xi_{3,f}=0 \tag{4.196}$$

$$.^0 \text{ terms}: \quad \xi_1\frac{\partial h}{\partial \lambda}+\xi_3\frac{\partial h}{\partial t}=\Big(\frac{\partial \eta_1}{\partial f}-\frac{\partial \xi_3}{\partial t}\Big)h+\frac{\partial \eta_1}{\partial t} \tag{4.197}$$

From the equations (4.194) and (4.195), it follows that ξ_1 is independent of t and f. Therefore, we obtain $\xi_1=\xi_1(\lambda,\mu,v)$. Moreover, equation (4.196) yields ξ_3 is independent of f, i.e. $\xi_3=\xi_3(\lambda,\mu,t,v)$. The equation (4.197) is a first order hyperbolic PDE satisfied by the source function $h(\lambda,t)$. This equation gives the family of source terms for which solutions of the equation $\mathcal{F}_1\equiv 0$ that are left invariant by the group of transformations exist, i.e. group invariant or similarity solutions exist.

Furthermore, the analysis of the nonlocal terms **(NLT)** reduces to solving the following nonlocal determining equation for the generators of the group of transformations:

$$\begin{aligned}\mathbf{NLT}:\quad \frac{1}{2}Y'(t)\,e^{-(Y(t)+\alpha_0\,\sigma)}\,T(f,v)\,\xi_3+\Big(\frac{\partial \eta_1}{\partial f}-\frac{\partial \xi_3}{\partial t}\Big)\Big(\frac{1}{2}\,e^{-(Y(t)+\alpha_0\,\sigma)}\,T(f,v)\Big)&\\ -\frac{1}{2}\,P_T(f,v)\,e^{-(Y(t)+\alpha_0\,\sigma)}=0.&\end{aligned} \tag{4.198}$$

If we multiply (4.198) by $2\,e^{Y(t)+\alpha_0\,\sigma}$ then equation (4.198) becomes

$$P_T(f,v)=T(f,v)\,\Big(Y'(t)\,\xi_3+\frac{\partial \eta_1}{\partial f}-\frac{\partial \xi_3}{\partial t}\Big). \tag{4.199}$$

Consequently, the system of equations (4.194 - 4.197) and (4.199) gives the first set of determining equations for the generators that are obtained from the invariance criterion of the equation $\mathcal{F}_1=0$ in the system of PIDEs (4.179).

The invariance condition for Eq. $\mathcal{F}_2 = 0$

Using (4.190) and the definition of $\mathcal{F}_2$, η_2^λ and η_2^μ we obtain the second determining equation in the form

$$G_T^{(1)}(\mathcal{F}_2) = 0 \quad \Rightarrow \quad \eta_2^\lambda + \eta_2^\mu = 0. \qquad \text{So,}$$

$$\frac{\partial \eta_2}{\partial \lambda} + \frac{\partial \eta_2}{\partial \mu} + \left(\frac{\partial \eta_2}{\partial v} - \frac{\partial \xi_1}{\partial \lambda}\right) v_\lambda + \left(\frac{\partial \eta_2}{\partial v} - \frac{\partial \xi_2}{\partial \mu}\right) v_\mu - \left(\frac{\partial \xi_3}{\partial \lambda} + \frac{\partial \xi_3}{\partial \mu}\right) v_t - \frac{\partial \xi_1}{\partial v} v_\lambda^2 - \frac{\partial \xi_1}{\partial v} v_\mu^2$$
$$- \frac{\partial \xi_3}{\partial v} v_\lambda \, v_t - \frac{\partial \xi_3}{\partial v} v_\mu \, v_t = 0 \qquad (4.200)$$

Similar to the analysis of the local term **LT** above, we solve (4.200) by splitting this term with respect to the local variables and their derivatives, and equating like derivatives to zero. We also make use of the equation $\mathcal{F}_2 = 0$ or $v_\mu = -v_\lambda$. Thus we obtain

$v_\lambda \, v_t$ terms: $\quad \xi_{3,v} = 0 \qquad (4.201)$

v_λ^2 terms: $\quad \xi_{1,v} = 0 \qquad (4.202)$

v_λ terms: $\quad \xi_{2,\mu} = \xi_{1,\lambda} \qquad (4.203)$

v_t terms: $\quad \xi_{3,\lambda} + \xi_{3,\mu} = 0 \qquad (4.204)$

$.^0$ terms: $\quad \eta_{2,\lambda} + \eta_{2,\mu} = 0 \qquad (4.205)$

From (4.196) and (4.201) we obtain $\xi_3 = \xi_3(\lambda, \mu, t)$, while from (4.194-4.195) and (4.202), we have $\xi_1 = \xi_1(\lambda, \mu)$. Next, we rewrite the nonlocal operator $P_T(f, v)$ in (4.192) as follows

$$P_T(f, v) = \int_0^\infty \theta \, v \, f \left\{ \frac{\xi_2 \, \beta(t) + \xi_3 \frac{\partial \theta}{\partial t}(\mu, t)}{\theta} + \frac{\eta_1}{f} + \frac{\eta_2}{v} + \frac{\partial \xi_2}{\partial \mu} + \frac{\partial \xi_2}{\partial f} f_\mu + \frac{\partial \xi_2}{\partial v} v_\mu \right\} d\mu. \qquad (4.206)$$

In addition, we assume that the term $\{...\}$ in (4.206) does not depend on μ so that it can be moved outside of the integral. This is equivalent to assuming that

$$\frac{\xi_2 \, \beta(t) + \xi_3 \frac{\partial \theta}{\partial t}(\mu, t)}{\theta}, \quad \frac{\eta_1}{f}, \quad \frac{\eta_2}{v}, \quad \frac{\partial \xi_2}{\partial \mu}, \quad \frac{\partial \xi_2}{\partial f} f_\mu, \quad \frac{\partial \xi_2}{\partial v} v_\mu$$

do not depend on μ. For simplicity, we assume that these are functions of t and also ξ_2 is independent of t, v and f. In view of the previous choices, the following identity holds

$$P_T(f,v) = A(t)\,T(f,v), \tag{4.207}$$

where $A(t)$ is an arbitrary function of t which will be defined below. As a result of (4.207), we obtain that the factor $Y'(t)\,\xi_3 + \eta_{1,f} - \xi_{3,t}$ in (4.199) is a function of t only. Thus, we get $Y'(t)\,\xi_3 + \eta_{1,f} - \xi_{3,t} = A(t)$. This means that ξ_3 is independent of λ and μ. On the other hand, due to the independence of f of the generators ξ_1 and since the equation (4.197) holds for all functions h, it follows that the generator η_1 must be a linear function of f with arbitrary constants as coefficients. In other words, based on (4.192), we have $\eta_1(f) = B_1\,f$.

4.3.5 Generators of the one-group of point transformations

Following the description in the previous section, we obtain:

(i) The following two relations for the generators ξ_2 and ξ_3 hold

$$\frac{\partial \xi_2}{\partial \mu} = C_3 \quad \text{and} \quad \beta(t)\,\xi_2(\mu) + \xi_3(t)\,\frac{\partial \theta}{\partial t}(\mu,t) = C_2\,\theta(\mu,t) \tag{4.208}$$

where C_2, C_3 are arbitrary constants. Of course, C_2 can be chosen as an arbitrary function of t. From the first relation in (4.208) and since (4.203) holds for all $\lambda, \mu \geq 0$, it seems reasonable to assume that $\xi_2 = \xi_2(\mu)$, and thus $\xi_1 = \xi_1(\lambda)$. In particular, we have $\xi_2(\mu) = C_3\,\mu + C_5$ and $\xi_1(\lambda) = C_3\,\lambda + C_4$, with C_4, C_5 arbitrary constants. Moreover, since the second equality in (4.208) also holds for all μ, $t \geq 0$ then using the definition of $\theta(\mu,t)$ we can set power-like terms in μ to zero. Thus, we obtain a coupled system of ODEs for the functions $\alpha(t)$ and $\beta(t)$ in the form

$$\xi_3(t)\,\beta'(t) = (C_2 - C_3)\,\beta(t) \tag{4.209}$$

$$\xi_3(t)\,\alpha'(t) - C_2\,\alpha(t) = -C_4\,\beta(t) \tag{4.210}$$

It is worth mentioning at this point that the only case of interest is $\xi_3(t) \neq 0$, for all $t \geq 0$. Otherwise, if $\xi_3(t) = 0$ then independent of the choice of the constants C_2 and C_3, the system (4.209, 4.210) has either a unique solution (trivial) $\alpha(t) = \beta(t) = 0$ or if $C_2 = C_3$ then $\alpha(t)$ and $\beta(t)$ are multiples of each other. Moreover, $\xi_3(t)$ will be determined from the equality that defines the operator P_T first by using its definition (4.192) and second by using the determining equation (4.199) that this satisfies. More precisely, using (4.208) then $\xi_3(t)$ satisfies the following equation

$$\int_0^\infty \Big\{C_2\,\theta(\mu,t)\,f\,v + B_1\,\theta(\mu,t)\,f\,v + \eta_2(t,v)\,\theta(\mu,t)\,f + C_3\,\theta(\mu,t)\,f\,v\Big\}\,d\mu$$
$$= T(f,v)\,\Big(Y'(t)\,\xi_3(t) + B_1 - \xi_3'(t)\Big) \tag{4.211}$$

(ii) To ensure both identities (4.207) and (4.205) are satisfied, we choose $\eta_2 = \eta_2(v,t) = B_2(t)\,v$, where $B_2(t)$ is an arbitrary function of t.

(iii) Using (4.211) and the information on η_2 in (ii) we obtain an ODE for $\xi_3(t)$

$$\xi_3'(t) - Y'(t)\,\xi_3(t) = A(t), \tag{4.212}$$

where $A(t) = -(C_2 + C_3 + B_2(t))$, with C_3, C_2 and $B_2(t)$ arbitrary.

Since we have the freedom to choose the function $B_2(t)$, then we will consider below two separate cases for which $\xi_3(t)$ can be determined explicitly. First, we discuss the simplest case $B_2(t) = B_2 =$ constant and provide a few similarity solutions. This first case will be identified as 4.3.6. Second, we choose $B_2(t) = B_3(t)\,\xi_3(t)$, where $B_3(t)$ is allowed to be arbitrary, yet we establish its dependence on the function $Y(t)$ to ensure the existence of similarity solutions to (4.176) which cannot be obtained otherwise (for instance, from 4.3.6 or any general function $B_2(t)$). We will identify the latter case as 4.3.7. Moreover, in each of the cases above, we determine the corresponding functions $\alpha(t)$ and $\beta(t)$, from the system of equations (4.209), (4.210).

4.3.6 Generator $\eta_2 = \eta_2(v) = B_2\,v$

In this case, the generators of the Lie group of point transformations admitted by the system (4.179) are given by:

$$\begin{aligned}
\xi_1 &= \xi_1(\lambda) = C_3\,\lambda + C_4\\
\xi_2 &= \xi_2(\mu) = C_3\,\mu + C_5\\
\xi_3 &= \xi_3(t)\\
\eta_1 &= \eta_1(f) = B_1\,f\\
\eta_2 &= \eta_2(v) = B_2\,v
\end{aligned}$$

where B_1, B_2, C_3, C_4, C_5 are arbitrary constants and $\xi_3(t)$ satisfies (4.212) and is given by

$$\xi_3(t) = A_2\, e^{Y(t)} - (C_2 + C_3 + B_2)\, e^{Y(t)} \int_0^t e^{-Y(\tau)}\, d\tau$$

where A_2 is an arbitrary constant. Consequently, the generators of the Lie group of point transformations admitted by the modified coagulation equation (4.176) are given by

$$\begin{aligned}
\xi_1(\lambda) &= C_3\,\lambda + C_4 \\
\xi_3(t) &= e^{Y(t)}\Big(A_2 - (A_1 + C_3)\, Z(t)\Big) \\
\eta_1(f) &= B_1\, f
\end{aligned}$$

where A_1, A_2, B_1, C_3, C_4 are arbitrary constants, and for simplicity we denote by $A_1 = B_2 + C_2$ and $Z(t) = \int_0^t e^{-Y(\tau)}\, d\tau$. The infinitesimal generator X associated with the Lie group of point transformations above can be written as

$$\begin{aligned}
X &= \xi_1(\lambda)\,\frac{\partial}{\partial\lambda} + \xi_3(t)\,\frac{\partial}{\partial t} + \eta_1(f)\,\frac{\partial}{\partial f} \\
&= A_2\, e^{Y(t)}\,\frac{\partial}{\partial t} + B_1\, f\,\frac{\partial}{\partial f} + A_1\Big(-Z(t)\, e^{Y(t)}\,\frac{\partial}{\partial t}\Big) + C_3\Big(\lambda\,\frac{\partial}{\partial\lambda} - Z(t)\, e^{Y(t)}\,\frac{\partial}{\partial t}\Big) + C_4\,\frac{\partial}{\partial\lambda}.
\end{aligned}$$

Therefore, the coagulation equation (4.176) has a five-parameter Lie group of transformations. More precisely, (4.176) admits a five-dimensional Lie algebra L_5 spanned by the following five Lie symmetry vector fields $V_1, ..., V_5$:

$$V_1 = e^{Y(t)}\,\frac{\partial}{\partial t},\quad V_2 = f\,\frac{\partial}{\partial f},\quad V_3 = -Z(t)\, e^{Y(t)}\,\frac{\partial}{\partial t},\quad V_4 = \lambda\,\frac{\partial}{\partial\lambda} - Z(t)\, e^{Y(t)}\,\frac{\partial}{\partial t},$$
$$V_5 = \frac{\partial}{\partial\lambda}. \tag{4.213}$$

These operators form a basis for the corresponding Lie algebra L_5. Similar, as in Section 4.2, we construct the commutator table for the Lie algebra arising from the infinitesimal generators V_i, where $i = 1, 2, ..., 5$, in Table 4.6.

Symmetry reductions for the coagulation equation

In order to obtain the similarity reductions for the coagulation equation (4.176), we have to solve first the corresponding characteristic equations in the invariant surface

$[V_i, V_j]$	V_1	V_2	V_3	V_4	V_5
V_1	0	0	$-V_1$	$-V_1$	0
V_2	0	0	0	0	0
V_3	V_1	0	0	0	0
V_4	V_1	0	0	0	$-V_5$
V_5	0	0	0	V_5	0

Table 4.6: Commutator $[V_i, V_j]$ table for the Lie algebra spanned by V_i and V_j in (4.213).

condition (4.45)

$$\frac{d\lambda}{\xi_1(\lambda)} = \frac{dt}{\xi_3(t)} = \frac{df}{\eta_1(f)}$$

associated to the generators ξ_1, ξ_3, η_1. Using the explicit forms of the generators above we obtain

$$\frac{d\lambda}{C_3\,\lambda + C_4} = \frac{Z'(t)\,dt}{A_2 - (B_2 + C_2 + C_3)\,Z(t)} = \frac{df}{B_1\,f} \tag{4.214}$$

As is the case with the Lie symmetry method, the solution of (4.214) involves two arbitrary constants, one of which plays the role of the similarity variable s and the other one plays the role of the similarity profile $\psi(s)$ from which the similarity solution $f(\lambda, t)$ will be obtained.

There are two major differences in this section when compared to Section 4.2. First, when solving for the similarity solution in this section, the substitution of the similarity solution $f(\lambda, t)$ into the original coagulation equation (4.176) results in an IDE for $\psi(s)$, instead of an ODE as in Section 4.2. Second, the solutions obtained by solving this IDE will generate directly the family of similarity solutions (or invariant solutions under the group of transformations) for the coagulation equation. In other words, we do not need to apply Laplace transforms to obtain the similarity solution c. In particular, we take the initial condition (4.177) into account and impose the invariance condition (4.45) for it. This reduces to imposing the invariance of $f(\lambda, t)$ along the curve $t = 0$ and using the original equation (4.176) to replace $f_t(\lambda, 0)$ in (4.45). In this way, we obtain particular solutions for the coagulation equation, which in some cases become exact, analytical solutions to (4.176) or (4.169).

We assume first that $C_3 \neq 0$ and treat the case $C_3 = 0$ separately. Moreover, we also assume $B_2 + C_2 + C_3 \neq 0$. In this case, the first and second pair of DEs in the characteristic equations (4.214) provide us with the similarity variable and similarity solution, respectively, in the form

$$s \equiv \left(\lambda + \frac{C_4}{C_3}\right) [R(t)]^b = \text{constant}, \quad \text{where } b = \frac{C_3}{B_2 + C_2 + C_3}$$

and

$$f(\lambda, t) = [R(t)]^a \, \psi(s), \quad \text{where } a = -\frac{B_1}{B_2 + C_2 + C_3} \tag{4.215}$$

with

$$R(t) = A_2 - (C_2 + C_3 + B_2) \int_0^t e^{-Y(\tau)} \, d\tau$$

where the constants A_2, B_2, C_2, C_3 are chosen such that $R(t) > 0$, for all $t \geq 0$.

It remains now to determine the type of source function $h(\lambda, t)$ for which similarity solutions to (4.176) exist. This follows from the equation (4.197) and using the expressions of ξ_1, ξ_3, η_1. We obtain

$$(C_3 \lambda + C_4) \frac{\partial h}{\partial \lambda}(\lambda, t) + e^{Y(t)} \Big[A_2 - (B_2 + C_2 + C_3) \, Z(t)\Big] \frac{\partial h}{\partial t}(\lambda, t) = \Big(B_1 - \xi_3'(t)\Big) \, h(\lambda, t).$$

Since this is a first order PDE then using the method of characteristics, we obtain that the source function $h(\lambda, t)$ takes the form

$$h(\lambda, t) = [R(t)]^{a-1} \, e^{-Y(t)} \, \varphi(s) \quad \text{where} \quad s \equiv \left(\lambda + \frac{C_4}{C_3}\right) [R(t)]^b. \tag{4.216}$$

To obtain group invariant solutions for (4.176), we have to proceed one more step, that is to substitute $f(\lambda, t)$, s and $h(\lambda, t)$ above into (4.176) and obtain the equation satisfied by the similarity profile $\psi(s)$ (which is in fact an ordinary IDE). For this purpose, we start by rewriting the convolution integral in (4.176), which for simplicity we denote as **RHS**, using the form (4.215) of $f(\lambda, t)$

$$\begin{aligned} \mathbf{RHS} = \frac{1}{2} e^{-(Y(t) + \alpha_0 \sigma)} [R(t)]^{2a-b} \int_{\frac{C_4}{C_3} [R(t)]^b}^{s} & \psi(s - s') \, \psi(s') \Big\{\alpha(t) + \beta(t) \, (s - s') \, [R(t)]^{-b}\Big\} \\ & \times \left\{\alpha(t) + \beta(t) \left(s' \, [R(t)]^{-b} - \frac{C_4}{C_3}\right)\right\} ds' \end{aligned} \tag{4.217}$$

On the other hand, substituting $f(\lambda, t)$ into the left-hand side we obtain

$$\begin{aligned} f_t &= R'(t) \, [R(t)]^{a-1} \, \{a\psi(s) + b \, s \, \psi'(s)\} \\ &= -(C_2 + C_3 + B_1) \, e^{-Y(t)} \, [R(t)]^{a-1} \, \{a\psi(s) + b \, s \, \psi'(s)\}. \end{aligned} \tag{4.218}$$

From (4.217), (4.218) and (4.216), we obtain

$$-\,(C_2+C_3+B_1)\,[R(t)]^{a-1}\,\{a\psi(s)+b\,s\,\psi'(s)\}=\frac{1}{2}\,e^{-\alpha_0\,\sigma}\,[R(t)]^{2a-b}\int_q^s\psi(s-s')$$
$$\times\,\psi(s')\left\{\alpha(t)+\beta(t)\,(s-s')\,[R(t)]^{-b}\right\}\left\{\alpha(t)+\beta(t)\left(s'\,[R(t)]^{-b}-\frac{C_4}{C_3}\right)\right\}ds'$$
$$+\,[R(t)]^{a-1}\,\varphi(s) \tag{4.219}$$

where $q:=\frac{C_4}{C_3}\,[R(t)]^b$.

In order to obtain invariant solutions, we need to eliminate first the time dependence in the integral in (4.219). One possibility to achieve this would be to make $q=0$ so, $C_4=0$. Using this information, we return to the coupled system of ODEs (4.209, 4.210) for the functions $\alpha(t)$ and $\beta(t)$, from which we obtain the general solutions in the form:

$$\alpha(t)=\alpha_0\,e^{C_2\int_0^t\frac{1}{\xi_3(\tau)}\,d\tau}=\alpha_0\,[R(t)]^c\text{and}\quad\beta(t)=\beta_0\,e^{(C_2-C_3)\int_0^t\frac{1}{\xi_3(\tau)}\,d\tau}=\beta_0\,[R(t)]^{c+b} \tag{4.220}$$

where $c=\frac{-C_2}{C_2+C_3+B_2}$, use being made of the definitions of a, b and c, where $\alpha_0\geq 0$ and $\beta_0\geq 0$ are arbitrary constants.

Using the definitions of $\alpha(t)$ and $\beta(t)$ in (4.220), the **RHS** becomes

$$\textbf{RHS}=\frac{1}{2}\,e^{-\alpha_0\,\sigma}[R(t)]^{2a-b+2c}\int_0^s\psi(s-s')\,\psi(s')\Big[\alpha_0+\beta_0\,(s-s')\Big]\Big[\alpha_0+\beta_0\,s'\Big]\,ds' \tag{4.221}$$

Using (4.221) and since $-a\,(C_2+C_3+B_1)=B_1$ and $-b\,(C_2+C_3+B_1)=-C_3$ then the equation (4.219) reduces to the following

$$[R(t)]^{a-1}\,\{B_1\,\psi(s)-C_3\,s\,\psi'(s)\}=[R(t)]^{a-1}\,\varphi(s)$$
$$+\,\frac{1}{2}\,e^{-\alpha_0\sigma}\,[R(t)]^{2a-b+2c}\int_0^s\psi(s-s')\,\psi(s')\Big[\alpha_0+\beta_0\,(s-s')\Big]\Big[\alpha_0+\beta_0\,s'\Big]\,ds'. \tag{4.222}$$

From the equation (4.222), it follows that a necessary condition for invariant solutions solutions $f(\lambda,t)$ to (4.176) to exist is given by the following equality

$$a-b+2c=-1\quad\Rightarrow\quad B_2=B_1+C_2. \tag{4.223}$$

So, $c=\frac{b-a-1}{2}$. Therefore, the similarity profile $\psi(s)$ satisfies the following ordinary IDE

$$B_1\,\psi(s)-C_3s\psi'(s)=\frac{1}{2}e^{-\alpha_0\sigma}\int_0^s\big(\alpha_0+\beta_0(s-s')\big)\big(\alpha_0+\beta_0s'\big)\psi(s-s')\psi(s')ds'+\varphi(s)$$

Gathering all the results obtained so far, we conclude with the following

General similarity solutions for the coagulation equation

Proposition 4.1 *Assume the source function $h(\lambda, t)$ has the similarity form*

$$h(\lambda, t) = [R(t)]^{a-1}\, e^{-Y(t)}\, \varphi(s),$$

where $Y(t)$ is defined in (4.173) and $\varphi(s)$ is an arbitrary, non-negative function for all $s \geq 0$ and s denotes the similarity variable

$$s = \lambda\,[R(t)]^{b}, \quad \text{where} \quad b = \frac{C_3}{2\,C_2 + B_1 + C_3} \quad \text{and} \quad a = -\frac{B_1}{2\,C_2 + B_1 + C_3}$$

and the function $R(t)$ is given by

$$R(t) = A_2 - (2\,C_2 + B_1 + C_3)\int_0^t e^{-Y(\tau)}\, d\tau,$$

with A_2, C_2, B_1, C_3 arbitrary constants such that $R(t) > 0$, for every $t \geq 0$. Assume the coagulation kernel $K(\lambda, \mu, t)$ has the form

$$K(\lambda, \mu, t) = (\alpha(t) + \beta(t)\,\lambda)\,(\alpha(t) + \beta(t)\,\mu),$$

where the functions $\alpha(t)$ and $\beta(t)$ are given by

$$\alpha(t) = \alpha_0\left[R(t)\right]^{\frac{b-a-1}{2}} \quad \text{and} \quad \beta(t) = \beta_0\left[R(t)\right]^{\frac{3b-a-1}{2}} \tag{4.224}$$

with α_0, $\beta_0 \geq 0$ some arbitrary constants. Then the coagulation equation (4.176) has a similarity solution of the form

$$f(\lambda, t) = [R(t)]^{a}\, \psi(s),$$

where the similarity profile $\psi(s)$ satisfies the ordinary IDE:

$$B_1\,\psi(s) - \varphi(s) - C_3 s\psi'(s) = \frac{e^{-\alpha_0\sigma}}{2}\int_0^s \big(\alpha_0 + \beta_0(s - s')\big)\big(\alpha_0 + \beta_0\, s'\big)\psi(s - s')\psi(s')\, ds' \tag{4.225}$$

In addition, we assume the constants A_2, B_1, C_2, C_3 are such that the function $\psi(s)$ is non-negative for all $s \geq 0$.

In addition, the source function $g(\lambda, t)$ and the similarity solution $c(\lambda, t)$ are given by

$$g(\lambda, t) = h(\lambda, t)\, e^{-\Phi(\lambda, t)}\, e^{-(\alpha_0 + \beta_0\,\lambda)\,\sigma} \quad \text{and} \quad c(\lambda, t) = [R(t)]^{a}\, \psi(s)\, e^{-\Phi(\lambda, t)}\, e^{-(\alpha_0 + \beta_0\,\lambda)\sigma}$$

where $\Phi(\lambda, t)$ and $Y(t)$ are defined in (4.173).

Remark 4.10 *To illustrate a family of similarity solutions $c(\lambda, t)$, we consider first an example of similarity functions $\varphi(s)$ satisfying Proposition 4.1. Since the similarity profile $\psi(s)$ is a non-negative function of s, for any $s \geq 0$ we consider a family of functions $\varphi(s)$ of the form:*

$$\varphi(s) = H_0 \, \psi(s), \quad \textit{where } H_0 \geq 0 \textit{ is a non-negative constant.} \tag{4.226}$$

In particular, if $H_0 = 0$ then $h(\lambda, t) = 0$ and so, $g(\lambda, t) = 0$ corresponding to the sourceless case. The idea that we present below can be applied to more general examples of functions $\varphi(s)$, not necessarily depending on $\psi(s)$. Our aim is to make use of the Laplace transform method to determine analytically (if possible) the similarity profile $\psi(s)$. For this reason, the choice we make in (4.226) seems appropriate to pursue our goal. For the functions $\varphi(s)$ in (4.226), we present a few particular examples of coagulation kernels, for which we provide similarity solutions $c(\lambda, t)$ to the coagulation equation (4.169).

The coagulation kernels of interest to our analysis are as follows:

(a) $K(\lambda, \mu, t) = \alpha^2(t)$;

(b) $K(\lambda, \mu, t) = \beta^2(t) \, \lambda \, \mu$;

(c) $K(\lambda, \mu, t) = (\alpha_0 + \beta_0 \, \lambda) \, (\alpha_0 + \beta_0 \, \mu)$, where α_0, $\beta_0 > 0$ are some arbitrary constants,

and $\alpha(t)$ and $\beta(t)$ are given by (4.224). For these examples we have obtained similarity solutions $c(\lambda, t)$, which for some particular initial conditions (and thus special choices of constants) become analytical solutions.

Case I: Coagulation kernel $K(\lambda, \mu, t) = \alpha^2(t)$

Assume that $\alpha(t) > 0$ and $\beta(t) = 0$. Choose the parameters $\beta_0 = 0$, $\alpha_0 > 0$ and $\sigma = 0$. One can rescale the space and time variables in the coagulation equation and set $\alpha_0 = 1$. Using the assumptions above and the definitions (4.224), the coagulation kernel takes the form

$$K(\lambda, \mu, t) = \alpha^2(t) = R(t)^{b-a-1}.$$

The function $R(t)$ is given by

$$R(t) = A_2 - (2\,C_2 + B_1 + C_3) \int_0^t e^{-Y(\tau)}\, d\tau \tag{4.227}$$

where A_2, C_2, C_3 are some arbitrary constants s.t. $R(t) > 0$, for every $t \geq 0$ and using the definition (4.173) we have

$$Y(t) = \int_0^t \alpha^2(\tau)\, M_0(\tau)\, d\tau \quad \Rightarrow \quad M_0(t) = Y'(t)\,[R(t)]^{a+1-b}. \tag{4.228}$$

In this case, based on the assumption in (4.226) that $\varphi(s) = H_0\,\psi(s)$ then the IDE (4.225) for $\psi(s)$ takes the form

$$(B_1 - H_0)\,\psi(s) - C_3\, s\, \psi'(s) = \frac{1}{2} \int_0^s \psi(s - s')\,\psi(s')\, ds' \tag{4.229}$$

To determine the solutions of (4.229), we use the method of Laplace transforms. For this purpose, denote the Laplace transform of $\psi(s)$ by

$$G(z) = \mathcal{L}\{\psi(s)\}(z) = \int_0^z e^{-s\,z}\,\psi(s)\, ds$$

then applying the Laplace transform operator $\mathcal{L}$ to the equation (4.229) gives rise to a separable ODE for $G(z)$:

$$G'(z) = \frac{1}{2\,C_3\, z} \cdot G(z)\,\left[G(z) - 2\,\mu\right]$$

where $\mu = B_1 + C_3 - H_0$. The solution of this ODE can be obtained explicitly in the form

$$G(z) = \frac{2\,\mu}{1 - C\, z^{\mu/C_3}}$$

where C is an arbitrary integration constant. The constant C will be completely determined from the initial condition (4.177) of the coagulation equation as will be shown in Example 4.12 below. Based on the definition of $G(z)$ as a Laplace transform, we assume the following necessary conditions hold: the constant $C < 0$ and the function $r(z) = 1 - C\, z^{\mu/C_3}$ is absolutely monotonic for all $z > z_0$, for some constant z_0, ensuring the complete monotonicity of the function $G(z)$ for all $z > z_0$. One way to achieve the latter would be by assuming that $\mu/C_3 = 1$ and $C_3 > 0$. This condition gives $\mu = C_3$ and thus we have $B_1 + C_3 - H_0 = C_3$ from which we obtain $H_0 = B_1 \geq 0$. For simplicity, denote by $p = -1/C > 0$. Thus, we obtain $G(z) = \frac{-2\,C_3}{C}\,\frac{1}{z - 1/C}$ or $G(z) = \frac{2\,C_3\,p}{z+p}$.

Taking the inverse Laplace transform of $G(z)$ above, the similarity profile $\psi(s)$ is given explicitly by

$$\psi(s) = 2\,C_3\,p\,e^{-p\,s}$$

where C_3, $p > 0$ are arbitrary constants that depend on the initial condition (4.170), $f_0(\lambda) = c_0(\lambda)$ that one chooses initially for the coagulation equation.

Using the definitions in Proposition 4.1, we obtain the form of the source function $g(\lambda, t)$ to be

$$g(\lambda, t) = 2\,H_0\,C_3\,p\,[R(t)]^{a-1}\,e^{-2\,Y(t)}\,e^{-p\,R(t)^b\,\lambda} \tag{4.230}$$

Therefore, the coagulation equation (4.169) has a similarity solution of the form

$$c(\lambda, t) = 2\,C_3\,p\,[R(t)]^a\,e^{-p\,[R(t)]^b\,\lambda}\,e^{-Y(t)}, \tag{4.231}$$

where $p > 0$ arbitrary and $a = -\frac{H_0}{2\,C_2+H_0+C_3}$ and $b = \frac{C_3}{2\,C_2+H_0+C_3}$.

To complete 4.3.6, Case I we need only to determine the expression of $Y(t)$. This can be obtained from the expression of the zeroth moment of solution obtained on the one hand from the general form of the similarity solution in (4.231) and on the other hand from (4.228). As a result we get

$$M_0(t) = \int_0^\infty c(\lambda, t)\,d\lambda = 2\,C_3\,e^{-Y(t)}\,[R(t)]^{a-b} = Y'(t)\,[R(t)]^{a+1-b}.$$

The latter equality gives rise to an I.V.P. for $Y(t)$:

$$Y'(t) = e^{-Y(t)}\,\frac{2\,C_3}{R(t)} = e^{-Y(t)}\,[S(t)]^{-1}, \quad \text{subject to I.C.} \quad Y(0) = 0,$$

where, for simplicity we denote by

$$S(t) = \frac{R(t)}{2\,C_3} = \frac{A_2}{2\,C_3} - \frac{2\,C_2 + H_0 + C_3}{2\,C_3}\int_0^t e^{-Y(\tau)}\,d\tau$$

So,

$$S'(t) = -\frac{(2\,C_2 + H_0 + C_3)}{2\,C_3}\,e^{-Y(t)}.$$

Using the initial condition $Y(0) = 0$, we determine $e^{-Y(t)}$ in terms of $S(t)$

$$Y'(t) = \frac{-2\,C_3}{2\,C_2 + H_0 + C_3}\,\frac{S'(t)}{S(t)} \quad \Rightarrow \quad Y(t) = \frac{-2\,C_3}{2\,C_2 + H_0 + C_3}\,\ln\left(\frac{S(t)}{S(0)}\right)$$

Hence, we obtain

$$e^{-Y(t)} = \left[\frac{S(t)}{S(0)}\right]^{\frac{2C_3}{2C_2+H_0+C_3}} = \Big[S(t)\Big]^{2b} \frac{(2\,C_3)^{2b}}{(A_2)^{2b}}$$

and thus an I.V.P. for $S(t)$ in the form

$$S'(t)\,[S(t)]^{-\frac{2C_3}{2C_2+H_0+C_3}} = -\frac{(2\,C_2 + H_0 + C_3)}{2\,C_3}\,[S(0)]^{-\frac{2C_3}{2C_2+H_0+C_3}} \tag{4.232}$$

subject to the initial condition $S(0) = \frac{A_2}{2C_3}$. There are two cases to consider here in order to describe the general solution of (4.232).

(i) If $2\,C_2 + H_0 \neq C_3$ then the general solution of (4.232) is given by

$$S(t) = \frac{A_2}{2\,C_3}\left\{1 - \frac{2\,C_2 + H_0 - C_3}{A_2}\,t\right\}^{\frac{2C_2+H_0+C_3}{2C_2+H_0-C_3}} \tag{4.233}$$

where A_2, C_2 and C_3 are some arbitrary constants that depend on the initial condition of (4.176). If we denote by $r = -\frac{2C_2+H_0-C_3}{A_2}$ assume that $r > 0$ and set $A_2 = 2\,C_3$ then the function $S(t)$ becomes

$$S(t) = (1 + r\,t)^{\frac{r-1}{r}}.$$

(ii) If $2\,C_2 + H_0 = C_3$ then the general solution of (4.232) becomes

$$S(t) = S(0)\,e^{-\frac{t}{S(0)}} = \frac{A_2}{2\,C_3}\,e^{-\frac{2C_3}{A_2}\,t} \tag{4.234}$$

Similar as in (i), we set $A_2 = 2\,C_3$ and obtain $S(t) = e^{-t}$.

In both cases (i) and (ii) above, if we substitute $R(t) = 2\,C_3\,S(t)$ and $e^{-Y(t)}$ into (4.231) and (4.230) we obtain the following similarity solution

$$\begin{aligned} c(\lambda, t) &= 2\,C_3\,p\,R(t)^a\,e^{-p\,R(t)^b\,\lambda}\,e^{-Y(t)} \\ &= \frac{p\,\big(2\,C_3\big)^{a+2\,b+1}}{(A_2)^{2b}}\,\Big[S(t)\Big]^{a+2\,b}\,e^{-p\,(2\,C_3)^b\,S(t)^b\,\lambda} \end{aligned}$$

and source function

$$\begin{aligned} g(\lambda, t) &= 2\,H_0\,C_3\,p\,R(t)^{a-1}\,e^{-p\,R(t)^b\,\lambda}\,e^{-2\,Y(t)} \\ &= \frac{H_0\,p\,\big(2\,C_3\big)^{a+4\,b}}{(A_2)^{4b}}\,\Big[S(t)\Big]^{a+4\,b-1}\,e^{-p\,(2\,C_3)^b\,S(t)^b\,\lambda} \end{aligned}$$

As a result of (i) and (ii) and all the above, we have derived the following general similarity solutions (family) for the coagulation equation (4.169) with particle source terms:

Example 4.12 ***(New families of explicit solutions to the coagulation equation for a time-dependent kernel)***
(i) *Assume that the coagulation kernel is given by*

$$K(\lambda,\mu,t) = \frac{q}{m}\,(1+r\,t)^{\frac{(b-a-1)\,(r-1)}{r}}$$

where $r > 0,\ r \neq 1,\quad H_0 \geq 0,\ C_3 > 0$ *and*

$$a = -\frac{H_0}{2\,C_3\,(1-r)} \quad \text{and} \quad b = \frac{1}{2\,(1-r)}$$

and $m = p\,(2\,C_3)^{a+1} > 0$ *and* $q = p\,(2\,C_3)^{b} > 0$ *are some arbitrary constants. If the source function* $g(\lambda,t)$ *has the form*

$$g(\lambda,t) = a\,m\,(r-1)\,(1+r\,t)^{\frac{(a+4\,b-1)\,(r-1)}{r}}\,e^{-q\,\lambda\,(1+r\,t)^{\frac{b\,(r-1)}{r}}} \geq 0. \tag{4.235}$$

Then the coagulation equation (4.169) has an explicit (similarity) solution of the form

$$c(\lambda,t) = m\,(1+r\,t)^{\frac{(a+2\,b)\,(r-1)}{r}}\,e^{-q\,\lambda\,(1+r\,t)^{\frac{b\,(r-1)}{r}}\,\lambda}. \tag{4.236}$$

(ii) *Assume that the coagulation kernel is given by*

$$K(\lambda,\mu,t) = \frac{q}{m}\,e^{(a+\frac{1}{2})\,t}$$

where $a = -\frac{H_0}{2\,C_3} \leq 0$, *and* $H_0 \geq 0$, $C_3 > 0$, q, m *are arbitrary constants defined in (i). If the source function* $g(\lambda,t)$ *has the form*

$$g(\lambda,t) = -a\,m\,e^{-(a+1)\,t}\,e^{-q\,\lambda\,e^{-t/2}} \geq 0.$$

Then the coagulation equation (4.169) has an explicit solution of the form

$$c(\lambda,t) = m\,e^{-(a+1)\,t}\,e^{-q\,\lambda\,e^{-t/2}}. \tag{4.237}$$

In particular, when $t = 0$, we obtain the initial condition $c_0(\lambda) = m\,e^{-q\,\lambda}$ and thus a new analytical solution for the coagulation equation with sources. Furthermore, if we choose $m = q$ in (i) then we recover the analytical solution in [17].

Remark 4.11 *(Regarding the solution (4.236)) To check completely our result in (i), we also compare the solution (4.236) to the well-known explicit solution for the pure coagulation equation of M. Smoluchowski [99] for which* $K \equiv 1$. *For this purpose, we choose* $a + 1 = b$ *and* $H_0 = 0$ *then we get* $a = 0$. *So,* $g(\lambda,t) = 0$ *and* $q = m$.

Moreover, from the definitions of a *and* b *we obtain* $C_2 = 0$ *and* $b = 1$ *which yields* $r = 1/2$ *and thus the constant kernel* $K \equiv 1$. *Hence, we recover the well-known explicit solution (see e.g. [94])*

$$c(\lambda, t) = \frac{4\,m}{(2+t)^2}\, e^{-\frac{2\,m\,\lambda}{2+t}}$$

In particular, if $m = 1$ *the solution above is M. Smoluchowski's solution in 1916.*

Mass conservation property

Although in this case the coagulation kernel is a time-dependent function, K is independent of the particle sizes λ and μ. As is general the case with these kernels, it is expected that the mass conservation property holds for all time $t \geq 0$. This is indeed what happens. To confirm our expected result, we prove that the following equality holds

$$M_1(t) = M_1(0) + G(t) = M_1(0) + \int_0^t \int_0^\infty \lambda\, g(\lambda, \tau)\, d\lambda\, d\tau, \quad \forall t \geq 0 \tag{4.238}$$

where $G(t)$ is such that its derivative $G'(t)$ represents the mass of the source function $g(\lambda, t)$.

(i) Indeed, on the one hand, using (4.236) we calculate $M_1(t)$ and obtain

$$M_1(t) = \int_0^\infty \lambda\, c(\lambda, t) = \frac{m}{q^2}\,(1 + r\,t)^{\frac{a(r-1)}{r}} \quad \Rightarrow \quad M_1(0) = \frac{m}{q^2}.$$

On the other hand, using (4.235) we calculate $G(t)$ and obtain

$$G(t) = -\frac{m}{q^2} + \frac{m}{q^2}\,(1 + r\,t)^{\frac{a(r-1)}{r}}.$$

Therefore, as expected the conservation of mass (4.238) holds for all $t \geq 0$.

(ii) Similarly, in this case we obtain

$$M_1(t) = \frac{m}{q^2}\, e^{-a\,t}$$

and

$$G(t) = \frac{m}{q^2}\,(e^{-at} - 1)$$

So, the conservation of mass also holds for the solution (4.237).

Case II: Coagulation kernel $K(\lambda,\mu,t) = \beta^2(t)\,\lambda\,\mu$

Assume $\alpha(t) = 0$ and $\beta(t) > 0$. Next, let us choose the parameters $\alpha_0 = 0$, $\beta_0 > 0$ and $\sigma \neq 0$. One can rescale the space and time variables in the coagulation equation and set $\beta_0 = 1$. Using the assumptions above and the definitions (4.224), the coagulation kernel takes the form

$$K(\lambda,\mu,t) = \beta^2(t)\,\lambda\,\mu = [R(t)]^{3b-a-1}\,\lambda\,\mu.$$

The function $R(t)$ is given in this case by

$$R(t) = A_2 - (2\,C_2 + B_1 + C_3)\int_0^t e^{-Y(\tau)}\,d\tau \tag{4.239}$$

where $H_0 \geq 0$ and C_2, B_1 and C_3 are some arbitrary constants s.t. $R(t) > 0$, for every $t \geq 0$. Using the definition (4.173), we obtain

$$Y(t) = \int_0^t \alpha(\tau)\,M_1(\tau)\,d\tau = 0. \tag{4.240}$$

Thus, we obtain

$$R(t) = A_2 - (2\,C_2 + B_1 + C_3)\,t.$$

In this case, based on the assumption in (4.226) that $\varphi(s) = H_0\,\psi(s)$ then the IDE (4.225) for $\psi(s)$ becomes

$$(B_1 - H_0)\,\psi(s) - C_3\,s\,\psi'(s) = \frac{1}{2}\int_0^s (s-s')\,s'\,\psi(s-s')\,\psi(s')\,ds' \tag{4.241}$$

To determine the similarity profile $\psi(s)$ we apply again the method of Laplace transforms as in 4.3.6, Case I. Due to the form of the integrand in (4.241), we first multiply (4.241) by s and denote by $\omega(s) = s\,\psi(s)$. We obtain

$$(B_1 + C_3 - H_0)\,\omega(s) - C_3\,s\,\omega'(s) = \frac{s}{2}\int_0^s \omega(s-s')\,\omega(s')\,ds' \tag{4.242}$$

Next, we consider the Laplace transform of $\omega(s)$

$$W(z) = \mathcal{L}\{\omega(s)\}(z) = \int_0^\infty e^{-zs}\,\omega(s)\,ds.$$

Applying the Laplace operator $\mathcal{L}$ to the new IDE (4.242) and using the properties of the Laplace Transforms then we obtain as usual an ODE for $W(z)$ in the form

$$W'(z) = \frac{q\,W(z)}{W(z) + C_3\,z} \quad \text{where} \quad q = H_0 - B_1 - 2\,C_3. \tag{4.243}$$

Define $\mu := 1 - C_3/q$. If we assume that q, $\mu \neq 0$ then the solution of (4.243) satisfies also an algebraic equation of the form:

$$\frac{1}{\mu q} W(z)^{\mu} - z\, W(z)^{\mu-1} + A = 0, \tag{4.244}$$

where A is a constant of integration that depends on the initial condition (4.170). To study closely the algebraic equation (4.244), we rewrite this equation as follows

$$z = \frac{1}{\mu q} W(z) + \frac{A}{W(z)^{\mu-1}}$$

Taking the limit as $z \to \infty$ on both sides and using the definition of $W(z)$ as a Laplace transform to get $W(z) \to 0$, we obtain a necessary condition in the form $\mu > 1$, which gives $C_3/q < 0$.

Moreover, define $\mathcal{F}(W) := \frac{1}{\mu q} W + \frac{A}{W^{\mu-1}} - z$. Differentiating both sides w.r.t. W, we obtain $\mathcal{F}'(W) = \frac{1}{\mu q} + A\,(1-\mu)\, W^{-\mu}$. Define W_{cp} to be the critical point of $\mathcal{F}(W)$, i.e. W_{cp} satisfies the equation $W_{cp}^{\mu} = -\frac{1}{A\,(\mu q)\,(1-\mu)} > 0$. So, we obtain $A\,q > 0$. Moreover, we expect that the function $W(z) > 0$ for all values $z > z_0$ (where z_0 is an arbitrary constant). One way to achieve this would be by assuming $\mathcal{F}''(W) > 0$, i.e. $A\,\mu\,(\mu-1)\, W^{-\mu-1} > 0$ which yields $A > 0$. The latter guarantees that $q > 0$, and thus $C_3 < 0$ and $H_0 > B_1 + 2\,C_3$.

Particular choice of constants. Explicit solutions to (4.169)

To illustrate how the method of Laplace transforms helps us determine some exact solutions to (4.244) and thus exact solutions to the coagulation equation (4.169) and corresponding source terms g, we choose a particular value for μ for which (4.244) can be solved explicitly. Since $\mu > 1$, then if we choose $\mu = 2$ the equation (4.244) in $W(z)$ becomes quadratic and thus it can be solved analytically. Since $\mu = 2$ we obtain $q = -C_3 > 0$ and using the definition of q then we get $B_1 = H_0 - C_3$. Thus we obtain

$$\frac{1}{2q} W(z)^2 - z\, W(z) + A = 0 \quad \Rightarrow \quad W(z) = q\left(z - \sqrt{z^2 - \frac{2A}{q}}\right).$$

In this case, we can calculate explicitly the inverse Laplace transform of $W(z)$. We obtain the similarity profile $\psi(s)$ to be

$$\psi(s) = \frac{2\sqrt{A\,q}\, I_1\!\left(2\sqrt{\frac{A}{q}}\, s\right)}{s^2} \tag{4.245}$$

where I_1 represents the modified Bessel function of the first kind [1].

Therefore, we obtain the similarity solution f and the source function h as follows

$$f(\lambda, t) = [R(t)]^a \, \psi(s) \quad \text{and} \quad h(\lambda, t) = \frac{H_0}{R(t)} f(\lambda, t)$$

where $R(t) = A_2 - (2\,C_2 + H_0)\,t$, use being made of the equality $H_0 = B_1 + C_3$. The arbitrary constants A_2 and A will be determined from the initial condition (or from the invariance of the initial condition) and such that $R(t) > 0$, for all $t \geq 0$. Furthermore, using the expression of $\psi(s)$ in (4.245) we obtain that the similarity solution $f(\lambda, t)$ and source term $h(\lambda, t)$ above take the form

$$f(\lambda, t) = 2\sqrt{q\,A}\, \frac{I_1\Big(2\sqrt{\frac{A}{q}}\, [R(t)]^b\, \lambda\Big)}{\lambda^2}\, [R(t)]^{a-2b} \quad \text{and} \quad h(\lambda, t) = \frac{H_0}{R(t)} f(\lambda, t).$$

Moreover, using the definitions (4.173) and since $N(t) = \beta(t)\, M_1(t)$, we get

$$\Phi(\lambda, t) = \int_0^t \lambda\, \beta^2(\tau)\, M_1(\tau)\, d\tau = \lambda \int_0^t [R(\tau)]^{3b-a-1}\, M_1(\tau)\, d\tau = \lambda\, V(t),$$

where for simplicity, we denote by

$$V(t) = \int_0^t [R(\tau)]^{3b-a-1}\, M_1(\tau)\, d\tau \quad \Rightarrow \quad M_1(t) = V'(t)\, [R(t)]^{a+1-3b}. \tag{4.246}$$

Finally, these notations and the definitions (4.175) yield the general similarity solution $c(\lambda, t)$ and the source term $g(\lambda, t)$ for (4.169) in the form

$$c(\lambda, t) = \frac{p\, I_1\Big(m\, [R(t)]^b\, \lambda\Big)}{\lambda^2\, [R(t)]^{2b-a}}\, e^{-\lambda(\sigma + V(t))} \quad \text{and} \quad g(\lambda, t) = \frac{H_0}{R(t)}\, c(\lambda, t) \tag{4.247}$$

where

$$p = 2\sqrt{A\,q} \quad \text{and} \quad m = 2\sqrt{\frac{A}{q}}$$

where $m, p > 0$ are some arbitrary constants and $R(t) = A_2 - (2\,C_2 + H_0)\,t$.

It is worth mentioning at this point, based on the form of the solution $\psi(s)$ obtained in (4.245) for $\mu = 2$, that for large $s \to \infty$ the convolution integral in (4.241) diverges. This is due to the fact that $\psi(s)$ in (4.245) develops a tail of the form $e^{2\sqrt{\frac{A}{q}}\, s}\, s^{-5/2}$ as $s \to \infty$, since for a large argument we have $I_1(x) \sim \frac{e^x}{\sqrt{2\pi x}}$, as $x \to \infty$. We have also performed an asymptotic large size behaviour ($s \to \infty$) for the similarity profile $\psi(s)$ for a general $\mu > 1$ (based on Newton's polygon method), however the analysis shows that again the function $\psi(s)$ has a tail $\psi(s) \sim e^{2\sqrt{\frac{A}{q}}\,s}\, s^{-5/2}$ as $s \to \infty$. Furthermore, these similarity solutions have the property that their similarity profile $\psi(s)$ have an infinite mass, in the sense that

$$\Phi_1 = \int_0^\infty s\,\psi(s)\,ds = \sqrt{\frac{2\,A\,q}{\pi}} \int_0^\infty e^{2\sqrt{\frac{A}{q}}\,s}\, s^{-3/2}\,ds = \infty.$$

However, in spite of the properties of the function $\psi(s)$, the similarity solution $c(\lambda, t)$ given by (4.247) to the coagulation equation (4.169) has finite mass $M_1(t) < \infty$, for all time $t \geq 0$. Moreover, due to the presence of the exponential decaying factor $e^{-(\sigma+V(t))\,\lambda}$, the solution $c(\lambda, t)$ in (4.247) is well-defined, for all λ, $t \geq 0$.

Based on the argument presented above, we proceed further to determine the solution $c(\lambda, t)$ in (4.247) completely, that is we obtain the function $V(t)$. For this purpose, first we make use of the similarity solution $c(\lambda, t)$ and the first moment of the solution $M_1(t)$ and since $q = p/m$, we obtain

$$M_1(t) = \frac{q}{R(t)^{3b-a}} \left\{ \sigma + V(t) - \sqrt{(\sigma + V(t))^2 - m^2\, R(t)^{2b}} \right\} = V'(t)\, R(t)^{a-3b+1}$$

use being made of (4.246). The last equality gives rise to an IVP for the unknown function $V(t)$

$$V'(t) = \frac{q}{R(t)} \left\{ \sigma + V(t) - \sqrt{(\sigma + V(t))^2 - m^2\, [R(t)]^{2b}} \right\} \quad \text{subject to I.C.} \quad V(0) = 0, \tag{4.248}$$

where $R(t) = A_2 - (2\,C_2 + H_0)\,t$, with the constants A_2, C_2 depending on the initial condition that one chooses for the problem. Having determined $V(t)$, then we can completely determine the solution $c(\lambda, t)$.

In the following we provide a few examples of initial conditions for which we derive exact similarity solutions. These initial conditions are obtained from the similarity solution (4.247) when we set $t = 0$. With the first example we recover the solution of Ernst et al [34], while the second example is a completely new explicit solution. Our both solutions are general (similarity) solutions which depend on the function $V(t)$. The latter satisfies an I.V.P. which in some cases can be solved analytically, however in general numerical methods need to be employed. The expression of $V(t)$ yields the total mass $M_1(t)$ for all time $t \geq 0$ and eventually the formula for the gel-time T_{gel}.

Case II. A: Coagulation kernel $K(\lambda,\mu,t) = \lambda\,\mu$

If we assume $a+1 = 3\,b$, then from the definitions of a and b and since $B_1 = H_0 - C_3$, we get $C_3 = C_2$. In addition, from (4.246), we get $V(t) = Q(t)$. Moreover, in this case the coagulation kernel $K(\lambda,\mu) = \lambda\,\mu$. We have obtained the following explicit solution to (4.169).

Example 4.13 *Assume the initial condition to (4.169) is given by*

$$c_0(\lambda) = \frac{e^{-\lambda\sigma}}{\lambda} \quad \textit{with } \sigma > 0 \textit{ any real number.} \tag{4.249}$$

Suppose the coagulation kernel $K(\lambda,\mu) = \lambda\,\mu$ and the source function $g(\lambda,t) = 0$. Then the coagulation equation (4.169) has an exact (similarity) solution of the form

$$c(\lambda,t) = \frac{e^{-\lambda\,(Q(t)+\sigma)}\, I_1(2\sqrt{t}\,\lambda)}{\lambda^2\sqrt{t}} \tag{4.250}$$

where the function $Q(t)$ is given by

$$Q(t) = \begin{cases} \frac{t}{\sigma} & \textit{for } \; t \in [0, T_{gel}) \\ 2\sqrt{t} - \sigma & \textit{for } \; t \geq T_{gel} \end{cases}$$

and $T_{gel} = \sigma^2$ denotes the gelation-time. In addition, the total mass of the solution $M_1(t)$ is obtained as

$$M_1(t) = Q'(t) = \begin{cases} \frac{1}{\sigma} & \textit{for } \; t \in [0, T_{gel}) \\ \frac{1}{\sqrt{t}} & \textit{for } \; t \geq T_{gel} \end{cases}$$

In particular, if $\sigma = 1$ the solution (4.253) above reduces to the solution in Ernst et al. [34].

Proof. In order to determine the similarity solution to the coagulation equation (4.169) subject to (4.249) we need to obtain the particular values for all the constants in (4.247). This can be done on one hand by imposing the invariance of the solution $f(\lambda,t)$ along the curve $t = 0$ (see [13, 14]), on the other hand by using the expression (4.249) above.

First, we impose the invariance condition for the initial data $f(\lambda,0) = e^{\lambda\sigma}\, c_0(\lambda) = \frac{1}{\lambda}$ and we obtain

$$\xi_1(\lambda)\, f_\lambda(\lambda,0) + \xi_3(0)\, f_t(\lambda,0) = \eta_1(f(\lambda,0)). \tag{4.251}$$

Using $\xi_1(\lambda) = C_2\,\lambda$, $\xi_3(0) = R(0) = A_2$, $\eta_1(f_0(\lambda)) = B_1\, f_0(\lambda) = \frac{B_1}{\lambda}$ and $Q(0) = 0$, and also the expression of f_t from (4.176)

$$f_t(\lambda, 0) = \frac{1}{2}\int_0^\lambda (\lambda - \mu)\,\mu\, f(\lambda - \mu, 0)\, f(\mu, 0)\, d\mu + f(\lambda, 0)\,\frac{H_0}{R(0)} = \frac{\lambda}{2} + \frac{H_0}{A_2}\,\frac{1}{\lambda}$$

then (4.251) reduces to the simpler equation

$$\frac{A_2}{2}\lambda + (H_0 - C_2 - B_1)\,\frac{1}{\lambda} = 0$$

which holds for any $\lambda > 0$. Since we have $B_1 = H_0 - C_2$ then the above equation yields $A_2 = 0$. Also, we have $q = H_0 - B_1 - 2\,C_2 = -C_2$. Therefore, we obtain $a = \frac{C_2 - H_0}{H_0 + 2\,C_2}$ and $b = \frac{C_2}{H_0 + 2\,C_2}$. Moreover, $R(t) = -(H_0 + 2\,C_2)\,t$, with $C_2 < 0$. If, in addition we make the assumption that $H_0 + 2\,C_2 < 0$, or $0 \leq H_0 < -2\,C_2$ so that $R(t) > 0$, for all $t \geq 0$, then we obtain $b > 0$. Thus, the similarity solution becomes

$$c(\lambda, t) = \frac{p\, e^{-\lambda(Q(t) + \sigma)}\, I_1\!\left(m\, t^b \lambda\right)}{\lambda^2\, t^{1-b}} \tag{4.252}$$

where, for simplicity we denote by

$$m = 2\sqrt{\frac{A}{-C_2}}\,[-(H_0 + 2\,C_2)]^b \quad \text{and} \quad p = \frac{2\sqrt{-A\,C_2}}{[-(H_0 + 2\,C_2)]^{1-b}}.$$

It remains now to make use of the initial condition (4.249) to determine all the constants. First, let's calculate $c_0(\lambda)$, which in this case has the form

$$c_0(\lambda) = \frac{p\, e^{-\lambda\sigma}}{\lambda^2} \lim_{t \to 0^+} \frac{I_1\!\left(m\, t^b \lambda\right)}{t^{1-b}}$$

for $\lambda > 0$ arbitrary but fixed and $b > 0$ an arbitrary constant.
One can use the asymptotic behaviour of the modified Bessel function $I_1(\cdot)$, for small arguments in order to evaluate the limit above and obtains

$$\frac{I_1\!\left(m\, t^b \lambda\right)}{\lambda^2\, t^{1-b}} \sim \frac{m\, t^{2b-1}}{2\lambda} \qquad \text{for} \qquad t \to 0^+.$$

The only possible value for the constant b such that the limit is nonzero and finite, would be $b = 1/2$, which when combined with the definition of $b = \frac{C_2}{H_0 + 2\,C_2} = \frac{1}{2}$ gives the unique solution $H_0 = 0$ and thus, $a = 1/2$.

As a result of the argument above, the initial condition (4.249) gives rise to similarity solutions of the form (4.252) if and only if $g(\lambda, t) = 0$ (no source terms). Substituting $b = \frac{1}{2}$ into the expression of $c(\lambda, t)$ above we obtain

$$c(\lambda, 0) = \frac{m\, p\, e^{-\lambda\sigma}}{2\,\lambda} = \frac{2\,A\, e^{-\lambda\sigma}}{\lambda}$$

where we use $m\,p = 4\,A$. To match the initial condition above with (4.249) we need only to set $A = 1/2$.

To summarize so far, the initial condition (4.249) in this example leads to analytical solutions (of a similarity type) only for the case when no particle source terms are included into the coagulating system, so $g(\lambda, t) = 0$ (or $H_0 = 0$). In this case, we obtain $a = b = 1/2$, $q = -C_2$ and $R(t) = -2\,C_2\,t = 2\,q\,t > 0$ (since $C_2 < 0$). Hence, the similarity solution reads as

$$c(\lambda, t) = 2\sqrt{A}\,\frac{e^{-\lambda(Q(t)+\sigma)}\,I_1(2\sqrt{2\,A}\,\sqrt{t}\,\lambda)}{\lambda^2\sqrt{2\,t}} = \frac{e^{-\lambda(Q(t)+\sigma)}\,I_1(2\sqrt{t}\,\lambda)}{\lambda^2\sqrt{t}} \tag{4.253}$$

where we use $A = 1/2$ to obtain the explicit solution given by Ernst et al. [34], using the saddle point method. The advantage of our method is that we obtain the exact solution without any knowledge of the total mass. It can be seen from (4.253), that $c(\lambda, t)$ has the total mass incorporated as part of the solution, in the form of the function $Q(t)$. Consequently, the group symmetry method provides us with a more general form of a solution, that depends on $M_1(t)$. The latter is in fact determined as a solution of an I.V.P. and will occupy us below.

In order to determine the expression of the function $Q(t)$ for $H_0 = 0$ (sourceless case), we return to the I.V.P (4.248) which now reads

$$Q'(t) = \frac{Q(t) + \sigma - \sqrt{(Q(t) + \sigma)^2 - 4\,t}}{2\,t} \quad \text{subject to} \quad Q(0) = 0. \tag{4.254}$$

Denote by $v(t) := Q(t) + \sigma$, then $v(0) = \sigma > 0$. Thus, (4.254) becomes an I.V.P for $v(t)$

$$v'(t) = \frac{v(t) - \sqrt{v^2(t) - 4\,t}}{2\,t} \quad \text{subject to} \quad Q(0) = 0 \tag{4.255}$$

$$t\,[v'(t)]^2 - v(t)\,v'(t) + 1 = 0 \quad \Rightarrow \quad v''(t)\cdot(2\,t\,v'(t) - v(t)) = 0 \tag{4.256}$$

The equations in (4.256) hold for values of $t \in [0, t_c)$ such that

$$v^2(t) \geq 4\,t \quad \text{and} \quad v(t) - 2\,t\,v'(t) \geq 0, \tag{4.257}$$

where T_c denotes the upper bound of the solution of the system (4.257) above. Thus, for any $t \in [0, T_c)$ we have

$$v''(t) = 0 \quad \text{or} \quad v(t) = \frac{t}{\sigma} + \sigma \quad \Rightarrow \quad Q(t) = \frac{t}{\sigma} \quad \text{for} \quad t \in [0, T_c = \sigma^2)$$

by using $M_1(0) = \frac{1}{\sigma}$ and $v(0) = \sigma$. Therefore, $M_1(t) = Q'(t) = \frac{1}{\sigma}$.

Remark 4.12 *The critical time T_c above corresponds to the gelation time.*

Indeed, on one hand the gel time T_{gel} corresponds to the first instance t when the second moment of solution blows up, or $M_2(t) = u_x(0,t) \to -\infty$. On the other hand, using the definition of $u(x,t)$ as a Laplace transform of $\lambda\, c(\lambda, t)$, we obtain that T_{gel} satisfies the equation $v^2(t) = 4\,t$ or $(\frac{t}{\sigma} + \sigma)^2 = 4\,t$, so $(t - \sigma^2)^2 = 0$ which gives $T_{gel} = \sigma^2$, so $T_c = T_{gel} = \sigma^2$. Therefore, the expression obtained above for $Q(t)$ corresponds in fact to the pre-gelation regime (for $t \in [0, T_{gel})$).

In the post-gelation stage ($t \geq T_{gel}$), we no longer have $v''(t) = 0$, however in this case, $v(t)$ satisfies the ODE

$v'(t) = \dfrac{1}{2t}\, v(t)$ whose solution is $v(t) = k\sqrt{t}$, where $k > 0$ is an arbitrary constant.

Therefore, we obtain the function $Q(t) = k\sqrt{t} - \sigma$, for $t \geq T_{gel}$. To determine the constant k, we use as an initial condition for the ODE above, the function $v(t)$ obtained for $t \in [0, T_{gel})$ or $v(T_{gel}) = 2\,\sigma$, ensuring thus the continuity of the total mass $M_1(t)$ at $t = T_{gel}$. This means that $k\,\sigma - \sigma = \sigma$ or $k = 2$. Alternatively, one simply notices, that for $t \geq T_{gel}$, the function $v(t) = 2\sqrt{t}$ satisfies both the equation (4.255) and the I.C. $v(T_{gel}) = 2\,\sigma$.

Therefore, we obtain the expression of $Q(t)$ for $t \geq \sigma^2$ i.e. $Q(t) = 2\sqrt{t} - \sigma$ and thus $M_1(t) = Q'(t) = \frac{1}{\sqrt{t}}$. Therefore, the expressions of the function $Q(t)$ and the total mass $M_1(t)$ in Example 4.13 hold and thus our example is complete. □

Our next example is for a different initial condition that is obtained from the similarity solution when we set $t = 0$.

Example 4.14 *Assume the initial condition is given by*

$$c_0(\lambda) = \frac{k\, e^{-\lambda\sigma}\, I_1(m\,\lambda)}{\lambda^2} \tag{4.258}$$

where σ, k, $m > 0$ are arbitrary constants and $\sigma \geq m$. Suppose the coagulation kernel $K(\lambda, \mu) = \lambda\,\mu$.

(i) *If the source function is given by*

$$g(\lambda, t) = \frac{p\,(2\,b - 1)\,k\,e^{-\lambda(Q(t)+\sigma)}\, I_1\Big(m\,(1 + p\,t)^b\,\lambda\Big)}{\lambda^2\,(1 + p\,t)^{2-b}}. \tag{4.259}$$

Then the coagulation equation (4.169) has an exact (similarity) solution of the form

$$c(\lambda,t)=\frac{k\,e^{-\lambda\,(Q(t)+\sigma)}\,I_1\Big(m\,(1+p\,t)^b\,\lambda\Big)}{\lambda^2\,(1+p\,t)^{1-b}},\tag{4.260}$$

where $p>0$ and $b\geq\frac{1}{2}$ are arbitrary and the function $Q(t)$ satisfies the I.V.P.

$$Q'(t)=\frac{k}{m\,(1+p\,t)}\Big(Q(t)+\sigma-\sqrt{(Q(t)+\sigma)^2-m^2\,[1+p\,t]^{2b}}\Big)\quad \textit{subject to}\quad Q(0)=0.\tag{4.261}$$

(ii) In particular, if $g(\lambda,t)=0$, then the coagulation equation (4.169) has an exact (similarity) solution of the form

$$c(\lambda,t)=\frac{k\,e^{-\lambda\,(Q(t)+\sigma)}\,I_1\Big(m\,\sqrt{1+\frac{2\,k}{m}\,t}\,\lambda\Big)}{\lambda^2\,\sqrt{1+\frac{2\,k}{m}\,t}}\tag{4.262}$$

where k, σ, $m>0$ are arbitrary and the function $Q(t)$ can be obtained explicitly as

$$Q(t):=\begin{cases}\frac{k}{m}\,(\sigma-\sigma_0)\,t, & \textit{for}\ \ t\in[0,T_{gel})\\ m\sqrt{1+\frac{2k}{m}\,t}-\sigma & \textit{for}\ \ t\geq T_{gel}\end{cases}$$

where the gelation time is given by $T_{gel}=\frac{\sigma_0\,m}{k\,(\sigma-\sigma_0)}$ and $\sigma_0:=\sqrt{\sigma^2-m^2}$. In addition, the total mass of the solution $M_1(t)$ is obtained to be

$$M_1(t)=Q'(t)=\begin{cases}\frac{k}{m}\,(\sigma-\sigma_0) & \textit{for}\ \ t\in[0,T_{gel})\\ \frac{k}{\sqrt{1+\frac{2k}{m}\,t}} & \textit{for}\ \ t\geq T_{gel}\end{cases}$$

Remark 4.13 *In particular, if we choose $b=1$, $\sigma=a$, $p=1/q$ and $m=k\,q$ then we obtain the Example 4.5 in Section 4.2.*

Proof. *(i)* Indeed, from (4.247) it follows that the similarity solution $c(\lambda,t)$ at $t=0$ takes the form

$$c(\lambda,0)=\frac{2\,\sqrt{q\,A}\,e^{-\lambda\sigma}\,I_1\Big(2\,\sqrt{\frac{A}{q}}\,(A_2)^b\,\lambda\Big)}{(A_2)^{1-b}\,\lambda^2}$$

where q, $A_2\neq 0$. To determine the constants, we need to impose certain conditions such that $c_0(\lambda)$ above matches the initial condition (4.258). For this reason, we first choose A, A_2, C_2 as follows

$$\frac{2\,\sqrt{q\,A}}{(A_2)^{1-b}}=k\quad\text{and}\quad 2\,\sqrt{\frac{A}{q}}\,(A_2)^b=m.$$

Alternatively, we can impose the invariance condition for the initial data $f_0(\lambda)$ as in the previous two examples. Moreover, if we define

$$P(t) := \frac{R(t)}{A_2} = 1 - \frac{H_0 + 2\,C_2}{A_2}\,t, \quad \text{and} \quad p := -\frac{H_0 + 2\,C_2}{A_2} > 0,$$

then $P(t) = 1 + p\,t$. From the definitions of $b = \frac{C_2}{H_0 + 2\,C_2}$ and p above, it follows that

$$\frac{H_0}{A_2} = -\frac{2\,C_2}{A_2} - p = 2\,p\,b - p = p\,(2\,b - 1)$$

where we make the additional assumption that $b \geq 1/2$, so that $H_0/A_2 \geq 0$. Substituting all the above into the expressions (4.247) then the similarity solution $c(\lambda, t)$ and the source function $g(\lambda, t)$ take the form (4.260) and (4.259), respectively. It remains to show that the function $Q(t)$ satisfies the I.V.P. (4.261). Indeed, taking the Laplace transform $u(x,t)$ of $\lambda\, c(\lambda, t)$, we obtain

$$u(x,t) = \frac{k}{m\,(1 + p\,t)}\left(x + Q(t) + \sigma - \sqrt{(x + Q(t) + \sigma)^2 - m^2\,(1 + p\,t)^{2b}}\right)$$

and substituting $x = 0$ we get $u(0,t) = M_1(t) = Q'(t)$, which proves (i) holds. Therefore, the function $Q(t)$ satisfies the I.V.P. (4.261). In general, the equation (4.261) cannot be solved analytically and numerical methods have to be employed.

(ii) We present below the case $H_0 = 0$ which corresponds to $g(\lambda, t) = 0$, as this is the only case for which one obtains exact similarity solutions $c(\lambda, t)$ to (4.169). Assume the constant $H_0 = 0$, then we have $B_1 = q = -C_2$ and $p = -2\,C_2/A_2$ and thus $a = b = 1/2$. Therefore, the I.V.P. (4.261) becomes

$$Q'(t) = \frac{k}{m\,(1 + p\,t)} \cdot \left(Q(t) + \sigma - \sqrt{(Q(t) + \sigma)^2 - m^2\,(1 + p\,t)}\right) \text{subject to } Q(0) = 0$$

We can simplify the I.V.P for $Q(t)$ if we define $v(t) := Q(t) + \sigma$ and thus obtain an I.V.P. for $v(t)$ in the form

$$v'(t) = \frac{k}{m\,(1 + p\,t)} \cdot \left(v(t) - \sqrt{v^2(t) - m^2\,(1 + p\,t)}\right) \quad \text{subject to} \quad v(0) = \sigma. \tag{4.263}$$

For all values of $t \geq 0$ such that the following system of inequalities hold

$$v^2(t) \geq m^2\,(1 + p\,t) \quad \text{and} \quad k\,v(t) - m\,v'(t)\,(1 + p\,t) \geq 0 \tag{4.264}$$

we rewrite the differential equation in (4.263) as follows

$$2\,v''(t) \cdot \left(v'(t)\,m\,(1 + p\,t) - k\,v(t)\right) + [v'(t)]^2\,(m\,p - 2k) = 0 \tag{4.265}$$

Using the definitions of $p = -\frac{2C_2}{A_2}$ and $m = 2\sqrt{\frac{A}{q}}\,A_2^b$, and since $q = -C_2$, we obtain

$$m\,p = 2\sqrt{\frac{A}{q}}\,A_2^b\left(-\frac{2\,C_2}{A_2}\right) = 2\cdot\frac{2\sqrt{A\,q}}{A_2^{1-b}} = 2\,k$$

where we use the definition of k and the fact that $b = 1/2$. Then $p = \frac{2k}{m}$ and (4.265) takes the simpler form

$$2\,v''(t)\,\big[v'(t)\,m\,(1+p\,t) - k\,v(t)\big] = 0 \tag{4.266}$$

For all values of $t \in [0, T_c)$, where T_c is an upper bound of the solution to the system (4.264) above, we have $v''(t) = 0$. This gives us the solution

$$v(t) = \frac{k}{m}(\sigma - \sigma_0)\,t + \sigma \quad \Rightarrow \quad Q(t) = \frac{k}{m}(\sigma - \sigma_0)\,t, \quad \text{for} \quad t \in [0, T_c)$$

where using $v(t)$ above to solve the system (4.264), we obtain an upper bound as the critical time $T_c = \frac{\sigma_0\,m}{k\,(\sigma-\sigma_0)}$. The solution $v(t)$ above follows by using the I.C. $v(0) = \sigma$ and the expression of $M_1(0) = \int_0^\infty \lambda\,c_0(\lambda)\,d\lambda = \frac{k}{m}(\sigma - \sigma_0)$, where $\sigma_0 := \sqrt{\sigma^2 - m^2}$ with $\sigma \geq m > 0$. Therefore, for $t \in [0, T_c)$, we have $M_1(t) = Q'(t) = \frac{k}{m}(\sigma - \sigma_0)$.

Similar as in Example 4.13, we show that the critical time T_c in fact coincides with the gelation time. Indeed, from the definition of the gel time, T_{gel} corresponds to the first instance when the second moment of solution blows up or $M_2(t) = u_x(0,t) \to -\infty$ which gives us $v^2(t) = m^2\,(1 + p\,t)$ or

$$\left(\frac{k}{m}(\sigma - \sigma_0)\,t + \sigma\right)^2 - m^2\,p\,t = m^2$$

Then using the definition of σ_0, we obtain $\left(\frac{k}{m}(\sigma - \sigma_0)\,t - \sigma_0\right)^2 = 0$ which gives the root $t = T_{gel} = \frac{\sigma_0\,m}{k\,(\sigma-\sigma_0)}$. Therefore, the expression we obtained above for $Q(t)$ corresponds to the pre-gelation regime.

On the other hand, in the post-gelation stage ($t \geq T_{gel}$), we no longer have $v''(t) = 0$. Here, we have

$$\frac{v'(t)}{v(t)} = \frac{k}{m\,(1+p\,t)} \quad \Rightarrow \quad v(t) = C\,\sqrt{1+p\,t}, \text{ where } C \text{ is an arbitrary constant.}$$

It follows that $Q(t) = C\,\sqrt{1+p\,t} - \sigma$. To determine the constant C, we use as an initial condition the function $v(t)$ obtained in the pre-gelation stage or $v(T_{gel}) = \sigma_0 + \sigma$

to ensure the continuity of $M_1(t)$ at $t = T_{gel}$. Therefore, we obtain $C = m$ and since $p = \frac{2k}{m}$ then $v(t) = m\sqrt{1 + \frac{2k}{m}\, t}$, for $t \geq T_{gel}$. Therefore, we obtain the expression of $Q(t)$ for $t \geq T_{gel}$ i.e. $Q(t) = m\sqrt{1 + \frac{2k}{m}\, t} - \sigma$ and thus $M_1(t) = Q'(t) = \frac{k}{\sqrt{1+\frac{2k}{m}\, t}}$.

Thus we have obtained the similarity solution (4.260) with $Q(t)$ and $M_1(t)$ given as in (ii), and our example is now complete. □

Case II. B: Coagulation kernel $K(\lambda, \mu, t) = (1 + k\, t)^{3b-a-1}\, \lambda\, \mu$, where $k > 0$

Gelation phenomenon

In this subsection, we consider the example of a coagulation kernel that increases with the particle sizes λ and μ, however it is allowed to be time-dependent. As described above, for this kernel the similarity solution c and the source function g are given by the formulas (4.247). In the following, we assume $3b \neq a + 1$, and $k > 0$ are some arbitrary constants. If the time-dependent factor $(1 + k\, t)^{3b-a-1}$ of the kernel $K(\lambda, \mu, t)$ decays sufficiently rapidly with time, then the second moment of solution $M_2(t)$ remains finite, for all $t \geq 0$.

Conjecture 4.2 *The total mass is conserved for all time $t \geq 0$ and thus gelation does not occur as a result.*

For the remainder of this subsection, our main focus is to analyze the validity of this conjecture. For this reason, we investigate the circumstances under which the gelation phenomenon can be completely prevented. This reduces to analyzing the conditions satisfied by the exponent $3b - a - 1$ and thus conditions for a and b and the initial second moment $M_2(0)$ of the solution c. To investigate the onset of gelation we make use of the original coagulation equation (4.169) and determine the second moment of solution $M_2(t)$. Indeed, based on the form of the kernel K in this conjecture, one can derive an ODE for $M_2(t)$ in the form

$$\frac{dM_2(t)}{dt} = \frac{1}{2}\, M_2^2(t)\, (1 + k\, t)^{3b-a-1} \tag{4.267}$$

provided that the third moment of solution $M_3(t)$ is finite. Thus, one can derive an explicit formula for the second moment in the form

$$\frac{1}{M_2(t)} = \frac{1}{M_2(0)} - \frac{1 - (1 + kt)^{3b-a}}{2k(3b - a)} \tag{4.268}$$

Provided that $M_2(0)$ is small enough and $3b - a < 0$ then one can prove that $M_2(t) > M_2(0) > 0$ remains finite for all time $t \geq 0$. The latter is a consequence of the fact that the right-hand side of (4.268) is strictly positive for all time $t \geq 0$, if we assume that $3b - a < 0$.

To prove the conjecture completely, one also needs to investigate the expression of the first moment $M_1(t)$ and show that the conservation of mass property holds, i.e.

$$M_1(t) = M_1(0) + \int_0^t \int_0^\infty \lambda\, g(\lambda, s)\, d\lambda\, ds, \quad \forall t \geq 0 \tag{4.269}$$

Furthermore, one also has to investigate whether the usual gelation time (that is the first time t at which the conservation of mass property (4.269) breaks down) coincide with the blow up time of the second moment. The latter is only proved rigorously for the pure coagulation, for a few special cases of initial conditions and a multiplicative kernel $K(\lambda, \mu) = (\alpha + \beta\, \lambda)\, (\alpha + \beta\, \mu)$, α, $\beta \geq 0$ (see e.g. [34, 96]). However, we leave the last two points in the conjecture for future work.

Case III: Coagulation kernel $K(\lambda, \mu, t) = (\alpha_0 + \beta_0\, \lambda)\, (\alpha_0 + \beta_0\, \mu)$

In this case, we have $\alpha(t) = \alpha_0 > 0$ and $\beta(t) = \beta_0 > 0$. We choose $C_3 = C_2 = 0$. We have $B_2 = B_1 + C_2 = B_1$ and

$$a = -\frac{B_1}{2\, C_2 + B_1 + C_3} = -\frac{B_1}{B_1} = -1 \quad \text{and} \quad b = \frac{C_3}{2\, C_2 + B_1 + C_3} = 0$$

In addition, we choose the parameter $\sigma \geq 0$ to be any real number. Furthermore, in view of (4.173), we have

$$\Phi(\lambda, t) = (\alpha_0 + \beta_0\, \lambda)\, Q(t) \quad \text{and} \quad Y(t) = \alpha_0\, Q(t)$$

and thus the similarity variable and similarity solution take the form

$$s \equiv \lambda, \quad \text{and} \quad c(\lambda, t) = \frac{\psi(\lambda)}{R(t)}\, e^{-(\alpha_0 + \beta_0\, \lambda)\, (Q(t) + \sigma)} \tag{4.270}$$

Also, the source function is given by

$$g(\lambda, t) = [R(t)]^{-2}\, e^{-Y(t)}\, \varphi(\lambda) = \frac{\varphi(\lambda)}{R(t)^2}\, e^{-(2\, \alpha_0 + \beta_0\, \lambda)\, (Q(t) + \sigma)}$$

where $R(t)$ is given by $R(t) = A_2 - B_2 \int_0^t e^{-\alpha_0 Q(\tau)}\, d\tau$ and $\varphi(\lambda) > 0$ is an arbitrary, non-negative function for all $\lambda \geq 0$. In addition, $\psi(\lambda)$ satisfies the following IDE

$$B_2\, \psi(\lambda) - \varphi(\lambda) = \frac{1}{2}\, e^{-\alpha_0 \sigma} \int_0^{\lambda} \left[\alpha_0 + \beta_0\,(\lambda - \mu)\right] \left[\alpha_0 + \beta_0\, \mu\right] \psi(\lambda - \mu)\, \psi(\mu)\, d\mu, \tag{4.271}$$

where the constants A_2, B_2 are chosen such that the function $\psi(\lambda) > 0$, for all $\lambda \geq 0$ and $R(t) > 0$, for every $t \geq 0$. For simplicity, choose $\sigma = 0$.

Multiply (4.271) by $(\alpha_0 + \beta_0\, \lambda)$ and define $\omega(\lambda) = (\alpha_0 + \beta_0\, \lambda)\, \psi(\lambda)$, then

$$B_2\, \omega(\lambda) - (\alpha_0 + \beta_0\, \lambda)\, \varphi(\lambda) = \frac{1}{2}\, (\alpha_0 + \beta_0\, \lambda) \int_0^{\lambda} \omega(\lambda - \mu)\, \omega(\mu)\, d\mu \tag{4.272}$$

Next, we attempt to solve (4.272) explicitly (if possible) by using the method of Laplace transforms. Define $W(z) = \mathcal{L}\{\omega(\lambda)\}(z)$ and $H(z) = \mathcal{L}\{\varphi(\lambda)\}(z)$, then (4.272) reduces to an ODE in $W(z)$:

$$B_2\, W(z) - \alpha_0\, H(z) + \beta_0\, H'(z) = \frac{\alpha_0}{2}\, W^2(z) - \beta_0\, W(z)\, W'(z) \tag{4.273}$$

In particular, if $H(z) = 0$ (which corresponds to $\varphi(\lambda) = 0$), so $g(\lambda, t) = 0$, then we obtain

$$W'(z) = \frac{\alpha_0}{2\, \beta_0}\, W(z) - \frac{B_2}{\beta_0}$$

whose general solution is given by

$$W(z) = A\, e^{\frac{\alpha_0}{2\beta_0} z} - \frac{B_2}{\beta_0}$$

where A is the integration constant. From the definition of $W(z)$ as a Laplace transform, we obtain $A = 0$ which yields a constant function $W(z) = -\frac{B_2}{\beta_0}$ as a solution. Consequently in Case III, if there are no particle source terms in the system, then the coagulation equation (4.169) does not possess any similarity solutions of the form (4.270).

Next, we look for some particular examples of functions $H(z)$ so that we can solve the ODE explicitly to determine $W(z)$. One such possible choice for $H(z)$, for example would be $H(z) = p\, W(z)$, or $\varphi(\lambda) = p\, \omega(\lambda) = p\, (\alpha_0 + \beta_0\, \lambda)\, \psi(\lambda)$, where

$p > 0$ arbitrary. In this case, using the properties of Laplace transforms the equation (4.273) becomes a separable ODE of the form:

$$W'(z) = \frac{W(z)\left(\frac{\alpha_0}{2\beta_0}\, W(z) + \frac{\alpha_0\, p - B_2}{\beta_0}\right)}{W(z) + p}$$

whose solution satisfies the algebraic equation

$$\left(\frac{\alpha_0}{2}\, W(z) + \alpha_0\, p - B_2\right)^{\frac{2\,B_2 - \alpha_0\, p}{\alpha_0\, p}} = W(z)\, e^{-\frac{\alpha_0\, p - B_2}{\beta_0\, p}\, z}\, A. \tag{4.274}$$

Since $W(z) \to 0$ as $z \to \infty$, then we obtain some necessary conditions for the constants, as follows: $\alpha_0\, p - B_2 < 0$ and $A > 0$, we set $A = 1$ for simplicity. Thus, we obtain $\frac{2\,B_2 - \alpha_0\, p}{\alpha_0\, p} > 1$.

In particular, if $\frac{2\,B_2 - \alpha_0\, p}{\alpha_0\, p} = 2$, or $B_2 = \frac{3\,\alpha_0\, p}{2} > 0$, then (4.274) becomes a quadratic equation in $W(z)$ whose solution is given by

$$W(z) = \frac{2}{\alpha_0^2}\left\{e^{\frac{\alpha_0}{2\beta_0}\, z} + q - \sqrt{\left(e^{\frac{\alpha_0}{2\beta_0}\, z} + q\right)^2 - q^2}\right\} \tag{4.275}$$

where $q := \frac{\alpha_0^2\, p}{2} > 0$, and $\alpha_0,\, \beta_0 > 0$. Here, we have $R(t) = A_2 - \frac{3\,\alpha_0\, p}{2}\int_0^t e^{-\alpha_0\, Q(\tau)}\, d\tau$ where A_2 will be determined from the initial condition $f_0(\lambda)$ that one chooses.

It remains to determine the function $Q'(t) = N(t) = \alpha_0\, M_0(t) + \beta_0\, M_1(t)$. One possible way to determine $Q(t)$ would be through $W(z)$ using both its definition and its explicit formula. On one hand, from the definition of $W(z)$ as a Laplace transform we obtain

$$\begin{aligned} W(z) = {} & \alpha_0\, R(t)\, e^{\alpha_0\, Q(t)} \int_0^\infty c(\lambda, t)\, e^{-\lambda(z - \beta_0\, Q(t))}\, d\lambda \\ & + \beta_0\, R(t)\, e^{\alpha_0\, Q(t)} \int_0^\infty \lambda\, c(\lambda, t)\, e^{-\lambda(z - \beta_0\, Q(t))}\, d\lambda \end{aligned} \tag{4.276}$$

where we substitute $\psi(\lambda)$ in terms of the solution $c(\lambda, t)$. It can be seen that $W(z)$ in (4.276) reduces to a linear combination of $M_0(t)$ and $M_1(t)$ if we set $z = \beta_0\, Q(t)$. Then we obtain

$$W(\beta_0\, Q(t)) = (\alpha_0\, M_0(t) + \beta_0\, M_1(t))\, R(t)\, e^{\alpha_0\, Q(t)} = Q'(t)\ R(t)\, e^{\alpha_0\, Q(t)} \tag{4.277}$$

On the other hand, substituting $z = \beta_0\, Q(t)$ into the explicit formula (4.275), and equating this new form and (4.277), we obtain an I.V.P for $Q(t)$:

$$Q'(t)\ R(t)\, e^{\alpha_0\, Q(t)} = \frac{2}{\alpha_0^2}\left\{q + e^{\frac{\alpha_0}{2}\, Q(t)} - \sqrt{\left(q + e^{\frac{\alpha_0}{2}\, Q(t)}\right)^2 - q^2}\right\} \tag{4.278}$$

subject to the initial condition $Q(0) = 0$. Since $R'(t) = -B_2 e^{-\alpha_0 Q(t)} < 0$ and $R''(t) = B_2 \alpha_0 Q'(t) e^{-\alpha_0 Q(t)}$ then $e^{\alpha_0 Q(t)} = -\frac{B_2}{R'(t)}$ and $Q'(t) = -\frac{R''(t)}{\alpha_0 R'(t)}$ then (4.278) becomes

$$\frac{B_2}{\alpha_0} \frac{R''(t)}{R'(t)} \frac{R(t)}{R'(t)} = \frac{2}{\alpha_0^2} \left\{ q + \frac{\sqrt{B_2}}{\sqrt{-R'(t)}} - \sqrt{\left(q + \frac{\sqrt{B_2}}{\sqrt{-R'(t)}} \right)^2 - q^2} \right\}$$

If we denote by $y(t) = \sqrt{-R'(t)}$ and $v(t) = q + \frac{\sqrt{B_2}}{y(t)}$. then the I.V.P. above simplifies to a separable DE $\frac{y'(t)}{y(t)} = -\frac{v'(t)}{v(t)-q}$ where $v(0) = q + 1$ and $y(0) = \sqrt{-B_2}$. Integrating both sides w.r.t. t from 0 to t we obtain

$$v(t) + \sqrt{v^2(t) - q^2} + q \ln \Big((v(t) + \sqrt{v^2(t) - q^2}) \, (v(t) - q) \Big) = q^2 \ln(R(t)) + \text{Const.}$$

which in terms of $R(t)$ reads

$$\begin{aligned} q + \frac{\sqrt{B_2}}{\sqrt{-R'(t)}} + \sqrt{\left(q + \frac{\sqrt{B_2}}{\sqrt{-R'(t)}} \right)^2 - q^2} + q \ln \left[\left(q + \frac{\sqrt{B_2}}{\sqrt{-R'(t)}} \right) \frac{\sqrt{B_2}}{(q+1)\sqrt{-R'(t)}} \right] \\ = q^2 \ln[R(t)] + q + 1 + \sqrt{2q+1} \qquad (4.279) \end{aligned}$$

In principle, one solves the differential equation (4.279) for $R(t)$ and obtains an implicit equation for $Q(t)$ which is valid for all $t \geq 0$. However, finding analytically the inverse Laplace transform of the function $W(z)$ defined by (4.275) may not be straightforward as pointed out already in Example 4.11. Then one either obtains a series solution for $c(\lambda, t)$ by formally expanding the square root in $W(z)$ or an asymptotic behaviour as $\lambda \to \infty$. Since we have not obtained an expression for the function $Q(t)$ or the gel-time in this case, we will leave this subcase as an open problem for future work.

4.3.7 Generator $\eta_2 = \eta_2(t, v) = \xi_3(t)\, B_3(t)\, v$

In this case, the generators of the Lie group of point transformations admitted by the system (4.179) are given by:

$$\begin{aligned} \xi_1 &= \xi_1(\lambda) = C_3\, \lambda + C_4 \\ \xi_2 &= \xi_2(\mu) = C_3\, \mu + C_5 \\ \xi_3 &= \xi_3(t) \\ \eta_1 &= \eta_1(f) = B_1\, f \\ \eta_2 &= \eta_2(t, v) = B_3(t)\, \xi_3(t)\, v \quad \text{(where } B_3(t) \text{ is an arbitrary function of } t\text{)} \end{aligned}$$

where C_3, C_4, C_5, B_1 are arbitrary constants. Using (4.212) with $A(t) = -(C_2+C_3+B_2(t))$, where here we choose $B_2(t) = \xi_3(t)\,B_3(t)$, we obtain that $\xi_3(t)$ satisfies the ODE

$$\xi_3'(t) + \xi_3(t)\,(B_3(t) - Y'(t)) = -(C_2 + C_3)$$

whose solution is given by

$$\xi_3(t) = e^{-(R(t)-Y(t))}\left[A_2 - (C_2+C_3)\int_0^t e^{R(\tau)-Y(\tau)}\,d\tau\right]$$

$$\text{where} \quad R(t) = \int_0^t B_3(\tau)\,d\tau \quad \text{and} \quad A_2 \text{ is a constant of integration}$$

and $Y(t)$ was defined in (4.173).

Proceeding similarly as in 4.3.6, we consider $C_3 \neq 0$ and set $C_4 = 0$ to obtain invariant solutions. Consequently, the generators of the Lie group of point transformations admitted by the modified coagulation equation (4.176) are given by

$$\begin{aligned}
\xi_1(\lambda) &= C_3\,\lambda \\
\xi_3(t) &= A_2\,e^{-(R(t)-Y(t))} - (C_2+C_3)\,e^{-(R(t)-Y(t))}\int_0^t e^{R(\tau)-Y(\tau)}\,d\tau \\
\eta_1(f) &= B_1\,f
\end{aligned}$$

where A_2, B_1, C_2, C_3 are arbitrary constants. In this case, since

$$\int_0^t \frac{1}{\xi_3(\tau)}\,d\tau = \left(\frac{P(t)}{P(0)}\right)^{-\frac{1}{C_2+C_3}} \tag{4.280}$$

the functions $\alpha(t)$ and $\beta(t)$ are given by

$$\alpha(t) = \alpha_0\,[P(t)]^{-\frac{C_2}{C_2+C_3}} \quad \text{and} \quad \beta(t) = \beta_0\,[P(t)]^{-\frac{C_2-C_3}{C_2+C_3}} \tag{4.281}$$

where

$$P(t) = A_2 - (C_2+C_3)\int_0^t e^{R(\tau)-Y(\tau)}\,d\tau.$$

Symmetry reductions for the coagulation equation

In order to obtain the similarity reductions for the coagulation equation (4.176), we solve the correspondent characteristic equations in the invariant surface condition (4.45) associated to the generators ξ_1, ξ_3, η_1, which in this case become

$$\frac{d\lambda}{C_3\,\lambda} = \frac{Z'(t)\,dt}{A_2 - (C_2 + C_3)\,Z(t)} = \frac{df}{B_1\,f} \tag{4.282}$$

where $Z(t) = \int_0^t e^{R(\tau)-Y(\tau)}\,d\tau$. We only consider here the case of $C_3 \neq 0$. In addition, we assume $B_1 \neq 0$ and $C_2 + C_3 \neq 0$. With these assumptions, the first and second pair of DEs in the characteristic equations (4.282) provide us with the similarity variable and similarity solution, respectively, in the form

$$s \equiv \lambda\,[P(t)]^b = \text{constant} \quad \text{and} \quad f(\lambda, t) = [P(t)]^a\,\psi(s)$$

where $b = \frac{C_3}{C_2+C_3}$ and $a = -\frac{B_1}{C_2+C_3}$ and also

$$P(t) = A_2 - (C_2 + C_3) \int_0^t e^{R(\tau)-Y(\tau)}\,d\tau$$

where again the choice of the constants A_2, C_2, C_3 is made subject to I.C. that one chooses, and so that $P(t) > 0$, for every $t \geq 0$.

It remains now to determine the type of source function $h(\lambda, t)$ for which similarity solutions to (4.176) exist. This follows from the equation (4.197) and the specific expressions of ξ_1, ξ_3, η_1 in this case. We obtain

$$C_3\,\lambda\,\frac{\partial h}{\partial \lambda}(\lambda, t) + \xi_3(t)\,\frac{\partial h}{\partial t}(\lambda, t) = \Big[C_2 + C_3 + B_1 - \xi_3(t)\,Y'(t) + B_3(t)\,\xi_3(t)\Big]\,h(\lambda, t)$$

Since this is a first order PDE we use again the method of characteristics. We obtain the following form for the source function that will provide us with invariant solutions f for the coagulation equation

$$h(\lambda, t) = [P(t)]^{a-1}\,e^{R(t)-Y(t)}\,\varphi(s).$$

To obtain group invariant solutions for (4.176), we need to substitute $f(\lambda, t)$, s and $h(\lambda, t)$ above into (4.176) and perform similar calculations to those leading to (4.222) in 4.3.6. By doing so, and using the new definitions of a and b, and the new functions $\alpha(t)$ and $\beta(t)$ in (4.281), the equation (4.176) takes the form

$$\begin{aligned}[P(t)]^{a-1}\{B_1\psi(s) - C_3\,s\,\psi'(s)\}\,e^{R(t)} &= [P(t)]^{a-1}\,e^{R(t)}\,\varphi(s) \\ &+ \frac{1}{2}\,e^{-\alpha_0\,\sigma}\,[P(t)]^{2a-b+2d}\int_0^s \psi(s-s')\,\psi(s')\left[\alpha_0+\beta\,(s-s')\right](\alpha_0+\beta_0\,s')\,ds'\end{aligned} \tag{4.283}$$

where $d = -\frac{C_2}{C_2+C_3}$. From the equation (4.283), it follows that a necessary condition for invariant solutions solutions $f(\lambda, t)$ to (4.176) to exist is given by the following equality

$$e^{R(t)} = [P(t)]^{a-b+2d+1} \quad \Rightarrow \quad B_3(t) = \frac{a+d}{P(t)} \tag{4.284}$$

that holds for all $t \geq 0$, where for simplicity we disregard a possible constant factor that may be present in (4.284). The last equality in (4.284) holds by differentiating w.r.t. t and using $b - d = 1$. Thus, we choose $R(t)$ such that $R(t) = (a - b + 2d + 1)\,\ln(P(t)) = (a + d)\,\ln(P(t))$.

Furthermore, in this case the similarity profile $\psi(s)$ satisfies the following ordinary IDE

$$B_1\psi(s) - C_3 s\psi'(s) = \frac{1}{2}e^{-\alpha_0\,\sigma}\int_0^s (\alpha_0+\beta_0(s-s'))(\alpha_0+\beta_0 s')\psi(s-s')\psi(s')ds' + \varphi(s)$$

Our aim is to present a few examples of new similarity solutions $c(\lambda, t)$. For this purpose, we have considered the same class (4.226) of functions $\varphi(s)$ as in 4.3.6, that is

$$\varphi(s) = H_0\,\psi(s), \text{ where } \quad H_0 \geq 0 \text{ is a non-negative constant.}$$

The more general case of functions $\varphi(s)$ is left for future work. For such a family of functions $\varphi(s)$, the function $h(\lambda, t)$ takes the form

$$h(\lambda, t) = H_0\,[P(t)]^{a-1}\,e^{R(t)-Y(t)}\,\psi(s), \quad \text{where } H_0 \geq 0.$$

In the following we consider some of the particular coagulation kernels in 4.3.6, for which we provide new similarity solutions $c(\lambda, t)$ to the coagulation equation (4.169). As it will be shown below these similarity solutions cannot be obtained otherwise, for example by assuming that the function $B_2(t) = B_2$ is only a constant (see 4.3.6).

Case I: Coagulation kernel $K(\lambda,\mu,t)=1$

In this case, we have $\alpha(t)=1$ and $\beta(t)=0$. So, the constants are given by $\alpha_0=1$, $\beta_0=0$ and $C_2=0$. Using the definitions of a,b,d, we obtain $d=0$, $b=1$ and $a=-B_1/C_3$. In addition, we choose the parameter $\sigma=0$. Then, in view of the necessary condition (4.284) we obtain

$$e^{R(t)}=P(t)^a.$$

Also, the similarity variable and similarity solution become

$$s\equiv\lambda\,[P(t)]=\text{constant}\quad\text{and}\quad f(\lambda,t)=[P(t)]^a\,\psi(s),$$

and

$$P(t)=A_2-C_3\int_0^t e^{R(\tau)-Q(\tau)}\,d\tau$$

since here $Y(t)=Q(t)$. Moreover, the IDE for $\psi(s)$ becomes

$$(B_1-H_0)\,\psi(s)-C_3\,s\,\psi'(s)=\frac{1}{2}\int_0^s\psi(s-s')\,\psi(s')\,ds' \tag{4.285}$$

for which we apply again the method of Laplace transforms. Consider the Laplace transform of $\psi(s)$ to be $G(z)=\mathcal{L}\{\psi(s)\}(z)$. Then, same as in 4.3.6, Case I, we obtain a separable ODE for $G(z)$:

$$G'(z)=\frac{G(z)\,(G(z)-2\,\mu)}{2\,C_3\,z}\quad\text{where}\quad\mu=B_1+C_3-H_0\quad\Rightarrow\quad G(z)=\frac{2\,C_3\nu}{z+\nu}$$

where $\nu>0$ is an arbitrary constant that depends on the constant of integration. This constant will be completely determined from the initial condition for the coagulation equation. From the definition of $G(z)$ as a Laplace transform, it follows that $G(z)$ is completely monotonic for all $z>z_0$, where z_0 is some arbitrary constant (one can choose $z_0=-\nu$). One way to achieve this would be assuming $C_3=\mu>0$ which gives $B_1=H_0\geq 0$. This means that $a=-H_0/C_3<0$.

Next, taking the inverse Laplace transform we obtain the similarity profile $\psi(s)$ to be

$$\psi(s)=2\,C_3\,\nu\,e^{-\nu s}$$

from which we derive the similarity solution $f(\lambda,t)$ and the source term $h(\lambda,t)$ to be

$$f(\lambda,t)=2\,C_3\,\nu\,[P(t)]^{-\frac{B_1}{C_3}}\,e^{-\lambda\nu\,[P(t)]}\quad\text{and}\quad h(\lambda,t)=\frac{H_0}{P(t)}\,e^{R(t)-Q(t)}\,f(\lambda,t). \tag{4.286}$$

Example 4.15 ***(Initial condition*** $c_0(\lambda) = e^{-\lambda}$ ***see e.g. [17]).*** *Let the initial condition (4.170) to the equation (4.169) be* $c_0(\lambda) = e^{-\lambda}$*. Let the coagulation kernel* $K \equiv 1$.

Let $R(t)$ *be a non-decreasing, non-negative function for all* $t \geq 0$*, such that* $R(0) = 0$*. Set*

$$T(t) = \frac{2}{2 + \int_0^t e^{R(\tau)}\, d\tau}.$$

Assume the source term is

$$g(\lambda, t) = R'(t)\, T^2(t)\, e^{R(t) - \lambda T(t)}. \tag{4.287}$$

Then the similarity (exact) solution to the coagulation equation (4.169) is

$$c(\lambda, t) = T^2(t)\, e^{R(t) - \lambda T(t)}. \tag{4.288}$$

Proof. First, we impose the invariance condition (4.45) for the similarity solution $f(\lambda, t)$ along the curve $t = 0$ in a similar manner as in 4.3.6, Case II and obtain $A_2 = 2\,C_3$, with $m = 1$. Moreover, from (4.286) we calculate $f(\lambda, 0)$ and obtain $f(\lambda, 0) = 2\,C_3\,\nu[A_2]^a\, e^{-\nu A_2 \lambda}$. On the other hand, since we have $f_0(\lambda) = e^{-\lambda}$ we can set $2\,C_3\,\nu = 1$ and $A_2 = 1$. So, $C_3 = \frac{1}{2}$ and $\nu = 1$. Then the similarity solution $f(\lambda, t)$ in (4.286) takes the form

$$f(\lambda, t) = e^{-\lambda T(t)}\, [P(t)]^a = e^{-\lambda T(t)}\, e^{R(t)}, \quad \text{where} \quad T(t) = \frac{P(t)}{A_2} = \frac{2 - \int_0^t e^{R(\tau) - Q(\tau)}\, d\tau}{2}$$

where we make use of $[P(t)]^a = e^{R(t)}$ and $P(t) = T(t)$. From here we obtain $e^{R(t) - Q(t)} = -2\,T'(t)$. Moreover, we have $c(\lambda, t) = f(\lambda, t)\, e^{-Q(t)} = e^{-\lambda T(t)}\, e^{R(t) - Q(t)}$ and since $Q'(t) = N(t) = M_0(t)$, then we can calculate

$$Q'(t) = M_0(t) = \int_0^\infty c(\lambda, t)\, d\lambda = e^{R(t) - Q(t)} \int_0^\infty e^{-\lambda T(t)}\, d\lambda = -2\,\frac{T'(t)}{T(t)}$$

So, $Q'(t) = -2\,\frac{T'(t)}{T(t)}$ subject to $Q(0) = 0$ and $T(0) = 1$, which by integration w.r.t t gives rise to $e^{-Q(t)} = T^2(t)$ and $T(t)$ can then be rewritten as follows

$$2\,T(t) = 2 - \int_0^t e^{R(\tau)} [T(\tau)]^2\, d\tau \quad \Rightarrow \quad -\frac{T'(t)}{T^2(t)} = \frac{e^{R(t)}}{2} \quad \text{subject to} \quad T(0) = 1.$$

Therefore, we obtain a new form of function $T(t)$ in terms of $R(t)$

$$T(t) = \frac{2}{2 + \int_0^t e^{R(\tau)}\, d\tau} > 0.$$

Let us briefly show that the properties of $R(t)$ in this example hold. Indeed, since $T'(t) = -C_3\, e^{R(t)-Q(t)} < 0$ (as $C_3 > 0$) then from $R'(t) = a\,\frac{T'(t)}{T(t)} > 0$ it follows that $R(t) > R(0) = 0$. So, $R(t)$ is a non-decreasing, non-negative function for all $t \geq 0$ such that $R(0) = 0$. In addition, since $e^{R(t)-Q(t)} = -T'(t)/C_3$, and $T'(t)/T(t) = R'(t)/a$ then we obtain (4.287, 4.288), or

$$c(\lambda, t) = e^{R(t)-\lambda T(t)}\, e^{-Q(t)} = T^2(t)\, e^{R(t)-\lambda T(t)}$$

$$g(\lambda, t) = \frac{H_0}{T(t)}\, e^{R(t)-Q(t)}\, c(\lambda, t) = R'(t)\, c(\lambda, t) = R'(t)\, T^2(t)\, e^{R(t)-\lambda T(t)} \qquad \square$$

Mass conservation property

In this case, since the kernel $K(\lambda, \mu) = 1$ then we expect that the total mass $M_1(t)$ satisfies the equality

$$M_1(t) = M_1(0) + G(t) = M_1(0) + \int_0^t \int_0^\infty \lambda\, g(\lambda, \tau)\, d\tau\, d\lambda$$

Indeed, the equality above holds and we obtain the total mass to be given by

$$M_1(t) = e^{R(t)}.$$

In particular, if $R(t) = 0$ then we get $M_1(t) = M_1(0) = 1$. Moreover, in this case we recover the old solution given by M. Smoluchowski [99].

Case II: Coagulation kernel $K(\lambda, \mu, t) = \lambda\, \mu$

In this case, $\alpha(t) = 0$ and $\beta(t) = 1$. Thus, the constants are given by $\alpha_0 = 0$, $\beta_0 = 1$ and $C_3 = C_2$. Using the definitions of a, b, d, we obtain $b = 1/2$, $d = b - 1 = -1/2$ and $a = -B_1/(2C_2)$. In addition, we choose the parameter $\sigma > 0$ arbitrary. Then, in view of the necessary condition (4.284) we obtain

$$e^{R(t)} = [P(t)]^{(a-\frac{1}{2})} \quad \text{or} \quad R(t) = \int_0^t B_3(\tau)\, d\tau = \left(a - \frac{1}{2}\right) \ln[P(t)].$$

Also, in this case the similarity variable and similarity solution become

$$s \equiv \lambda\, [P(t)]^{1/2} = \text{constant} \quad \text{and} \quad f(\lambda, t) = [P(t)]^a\, \psi(s),$$

where

$$P(t) = A_2 - 2\, C_2 \int_0^t e^{R(\tau)}\, d\tau \quad \text{since} \quad Y(t) = 0.$$

Then the IDE equation for $\psi(s)$ reduces to

$$(B_1 - H_0)\,\psi(s) - C_2\, s\, \psi'(s) = \frac{1}{2} \int_0^s \psi(s - s')\, \psi(s')\, (s - s')\, s'\, ds' \tag{4.289}$$

where the same particular source function as in 4.3.6, Case II has been considered as an example for our analysis, that is $\varphi(s) = H_0\, \psi(s)$.

Since (4.289) is the same equation as (4.241) in 4.3.6, Case II, we refer to the details there. We obtain an ODE for the Laplace transform of $s\,\psi(s)$, that is for $W(z)$ in the form

$$\frac{1}{\mu q} W(z)^{\mu} - z\, W(z) + A = 0$$

where A is the constant of integration that depends on the initial condition (4.170) and $\mu = 1 - C_2/q$. For the same choice of constants as in 4.3.6, Case II, that is $\mu = 2$, we obtain an analytical solution to (4.169). This implies that $q = H_0 - B_1 - 2\,C_2 = -C_2 > 0$, so, $B_1 = H_0 - C_2$ and the solution $W(z)$ becomes

$$W(z) = q\left(z - \sqrt{z^2 - \frac{2\,A}{q}}\right).$$

whose inverse Laplace transform gives the similarity profile $\psi(s)$ explicitly as

$$\psi(s) = \frac{2\sqrt{A\,q}\, I_1\!\left(2\,\sqrt{\frac{A}{q}}\, s\right)}{s^2} \tag{4.290}$$

where I_1 represents the modified Bessel function of the first kind.

Therefore, the similarity solutions for the equations (4.176) and (4.169) take now the following form

$$f(\lambda, t) = [P(t)]^a\, \psi(s) \;\Rightarrow\; c(\lambda, t) = f(\lambda, t)\, e^{-(Q(t)+\sigma)\,\lambda} = [P(t)]^a\, e^{-(Q(t)+\sigma)\,\lambda}\, \psi(\lambda\, [P(t)]^{1/2})$$

The source functions for which such similarity solutions occur are given by

$$h(\lambda, t) = H_0 e^{R(t)} [P(t)]^{a-1} \psi(s) \quad \text{and} \quad g(\lambda, t) = \frac{H_0\, e^{R(t)}}{P(t)}\, c(\lambda, t)$$

where $a = -B_1/(2\,C_2)$ and $P(t) = A_2 - 2\,C_2 \int_0^t e^{R(\tau)}\, d\tau$. The arbitrary constants A_2 and A will be determined from the initial condition that one chooses to solve (4.169) and s.t. $P(t) > 0,\ \forall t \geq 0$.

Using the expression (4.290) for $\psi(s)$ we obtain the following similarity solution and source function

$$c(\lambda,t) = 2\sqrt{q\,A}\,\frac{e^{-\lambda\,(Q(t)+\sigma)}\,I_1\Big(2\sqrt{\tfrac{A}{q}\,P(t)}\,\lambda\Big)}{\lambda^2\,[P(t)]^{1-a}} \quad \text{and} \quad g(\lambda,t) = \frac{H_0\,e^{R(t)}}{P(t)}\,c(\lambda,t). \tag{4.291}$$

In the following we choose the same initial condition (4.258) as in Example 4.14 and derive some new similarity solutions to (4.169) however, this time in the presence of particle source terms.

Example 4.16 $\Big($***Initial condition*** $c_0(\lambda) = \frac{k\,e^{-\lambda\sigma}\,I_1(m\,\lambda)}{\lambda^2}\Big)$
(i) *Assume the initial condition to (4.169) is*

$$c_0(\lambda) = \frac{k\,e^{-\lambda\sigma}\,I_1(m\,\lambda)}{\lambda^2} \quad \textit{where } \sigma,\ k,\ m > 0 \textit{ are arbitrary constants.}$$

Assume the coagulation kernel $K(\lambda,\mu,t) = \lambda\,\mu$. *Let* $S(t) \geq 0$ *defined by*

$$S(t) = \Big[1 + \frac{k}{m}\,(3-2\,a)\,t\Big]^{\frac{2}{3-2a}}$$

where $a \geq 1/2$ *is an arbitrary constant. Assume the source function* $g(\lambda,t)$ *has the form*

$$g(\lambda,t) = H_0\,\frac{k\,e^{-\lambda\,(Q(t)+\sigma)}\,I_1(m\,\sqrt{S(t)}\,\lambda)}{\lambda^2}\,S(t)^{2a-5/2} \tag{4.292}$$

where $H_0 \geq 0$ *is an arbitrary constant. Then the coagulation equation (4.169) has an exact (similarity) solution of the form*

$$c(\lambda,t) = \frac{k\,e^{-\lambda\,(Q(t)+\sigma)}\,I_1(m\,\sqrt{S(t)}\,\lambda)}{\lambda^2\,[S(t)]^{1-a}} \tag{4.293}$$

where $Q(t)$ *satisfies the I.V.P.*

$$Q'(t) = \frac{k}{m\,S(t)^{3/2-a}}\Big(Q(t) + \sigma - \sqrt{(Q(t)+\sigma)^2 - m^2\,S(t)}\Big) \quad \textit{subject to} \quad Q(0) = 0. \tag{4.294}$$

(ii) *In particular, if* $a = 1$ *and* $H_0 = \frac{k}{m}$, *then the function* $S(t)$ *takes the form*

$$S(t) = \Big(1 + \frac{k}{m}\,t\Big)^2 > 0, \quad \forall t \geq 0.$$

If the source function $g(\lambda, t)$ *is given by*

$$g(\lambda, t) = \frac{k^2 \, e^{-\lambda(Q(t)+\sigma)} \, I_1((k\,t + m)\,\lambda)}{\lambda^2 \, (k\,t + m)} \tag{4.295}$$

Then the coagulation equation (4.169) has an exact (similarity) solution of the form

$$c(\lambda, t) = \frac{k \, e^{-\lambda(Q(t)+\sigma)} \, I_1((k\,t + m)\,\lambda)}{\lambda^2} \tag{4.296}$$

where the function $Q(t)$ *is given by*

$$Q(t) = \begin{cases} \frac{k}{m^2}\,(\sigma - \sigma_0)\left(\frac{k}{2}\,t^2 + m\,t\right), & \textit{for } \; t \in [0, T_{gel}) \\ k\,t + m - \sigma, & \textit{for } \; t \geq T_{gel} \end{cases}$$

and the gel-time is defined as $T_{gel} = \frac{m}{k}\left(\sqrt{\frac{\sigma+\sigma_0}{\sigma-\sigma_0}} - 1\right)$ *where* $\sigma_0 = \sqrt{\sigma^2 - m^2}$, $\sigma \geq m > 0$. *In addition, the total mass of the solution* $M_1(t)$ *is obtained as*

$$M_1(t) = Q'(t) = \begin{cases} \frac{k}{m^2}\,(\sigma - \sigma_0)\,(kt + m), & \textit{for } \; t \in [0, T_{gel}) \\ k, & \textit{for } \; t \geq T_{gel} \end{cases}$$

Remark 4.14 *Example 4.16 is a particular case of Example 4.14, where* $b = 1$ *and* $k = \frac{p}{m}$.

Proof. *(i)* Indeed, the similarity solution at $t = 0$ becomes

$$c(\lambda, 0) = \frac{2\,\sqrt{q\,A}\,e^{-\lambda\sigma}\,I_1\!\left(2\,\sqrt{\frac{A}{q}\,A_2}\,\lambda\right)}{(A_2)^{1-a}\,\lambda^2}$$

If we choose

$$\frac{2\sqrt{q\,A}}{(A_2)^{1-a}} = k \quad \text{and} \quad 2\,\sqrt{\frac{A}{q}\,A_2} = m \tag{4.297}$$

and set $S(t) = \frac{P(t)}{A_2} = 1 - \frac{2C_2}{A_2}\int_0^t e^{R(\tau)}\,d\tau$, where $C_2 < 0$ and $A_2 = 1$, then using (4.291) the similarity solution c and the source term g are given as in (4.293) and (4.292), respectively. From the definition of $R(t)$ we have $R(t) = (a - \frac{1}{2})\,\ln[P(t)]$ and since $P(0) = A_2 = 1$, then $R(0) = 0$. Moreover, since $a = -\frac{B_1}{2C_2}$ and $B_1 = H_0 - C_2$ then we obtain $a = -\frac{H_0}{2C_2} + \frac{1}{2}$, and with $-C_2 > 0$ and $H_0 \geq 0$, we obtain $a \geq 1/2$.

Using the notations (4.297), the form (4.291) for the solution $c(\lambda, t)$, and since $P(t) = S(t)$, we obtain

$$c(\lambda, t) = \frac{k\, e^{-\lambda(Q(t)+\sigma)}\, I_1(m\,\sqrt{S(t)}\,\lambda)}{\lambda^2\, S(t)^{1-a}}$$

From (4.297), and setting $A_2 = 1$, we obtain $q = -\frac{k}{m}$. On the other hand, we have $q = H_0 - B_1 - 2\,C_2$ and since $H_0 - B_1 = C_2$ then $q = -C_2$. Thus equating the above forms of q we get $-C_2 = \frac{k}{m}$. So,

$$S(t) = 1 - 2\,C_2 \int_0^t e^{R(\tau)}\, d\tau = 1 + \frac{2\,k}{m} \int_0^t e^{R(\tau)}\, d\tau$$

Then

$$S'(t) = \frac{2\,k}{m}\, e^{R(t)} = \frac{2\,k}{m}\, S(t)^{a-1/2},$$

which is a separable ODE for $S(t)$ with initial condition $S(0) = 1$, whose general solution is

$$S(t) = \Big(1 + \frac{k}{m}\,(3 - 2a)\,t\Big)^{\frac{2}{3-2a}}.$$

Then the source function $g(\lambda, t)$ in (4.291) takes the form

$$\begin{aligned} g(\lambda, t) = \frac{H_0\, e^{R(t)}}{S(t)}\, c(\lambda, t) \quad &\Rightarrow \quad g(\lambda, t) = H_0\, S(t)^{a-3/2}\, c(\lambda, t) \\ &= H_0\, \frac{k\, e^{-\lambda(Q(t)+\sigma)}\, I_1(m\,\sqrt{S(t)}\,\lambda)}{\lambda^2}\, S(t)^{2a-5/2} \end{aligned}$$

Thus (4.292) holds true. In particular, if $a = 1/2$ then we have $B_1 = -C_2$ which gives $H_0 = 0$ and thus we obtain the sourceless case $g(\lambda, t) = 0$ which has already been covered in Example 4.14. Moreover, since $P(t)$ and $P'(t) > 0$ it follows that $R(t)$ is a non-negative and non-decreasing function for all $t \geq 0$.

In addition, we obtain that the function $Q(t)$ satisfies the I.V.P.

$$Q'(t) = \frac{k}{m\, S(t)^{3/2-a}} \Big(Q(t) + \sigma - \sqrt{(Q(t) + \sigma)^2 - m^2\, S(t)}\Big), \quad \text{subject to} \quad Q(0) = 0. \tag{4.298}$$

In general, one cannot solve (4.298) to obtain $Q(t)$ analytically. There are a few particular choices that one can make to solve the DE and study the occurrence of gelation. One such example corresponds to the choice of $a = 1$.

(ii) Choose $a = 1$. So, $S(t) = \left(1 + \frac{k}{m}\,t\right)^2$. For simplicity, define $\varphi(t) = m\,\sqrt{S(t)} = k\,t + m$. Then we obtain, $H_0 = -C_2 > 0$ and thus $q = -C_2 = H_0$. Moreover, if we divide the equations (4.297) to each other then we obtain $q = H_0 = \frac{k}{m}$. Then the function $S(t)$ takes the form:

$$S(t) = 1 + \frac{2\,k}{m}\int_0^t e^{R(\tau)}\,d\tau > 0, \qquad \text{for all } t \geq 0.$$

Let's also denote by $v(t) := Q(t) + \sigma$. Then (4.298) becomes an I.V.P. for $v(t)$ of the form

$$v'(t) = \frac{k}{\varphi(t)} \cdot \left[v(t) - \sqrt{v^2(t) - \varphi^2(t)}\right] \quad \text{subject to} \quad v(0) = \sigma. \tag{4.299}$$

For values of $t \geq 0$ such that the following system of inequalities hold

$$v(t) \geq \varphi(t) \quad \text{and} \quad k\,v(t) - \varphi(t)\,v'(t) \geq 0, \tag{4.300}$$

we rewrite the equation (4.299) as follows

$$v'(t)^2 - \frac{2k\,v(t)\,v'(t)}{\varphi(t)} = -k^2$$

and by differentiating this equation w.r.t. t we obtain

$$\left(v''(t) - \frac{k}{\varphi(t)}\,v'(t)\right) \cdot \left(v'(t) - \frac{k}{\varphi(t)}\,v(t)\right) = 0.$$

From this equation we get two DEs

$$v''(t) - \frac{k}{\varphi(t)}\,v'(t) = 0 \tag{4.301}$$

and

$$v'(t) - \frac{k}{\varphi(t)}\,v(t) = 0 \tag{4.302}$$

It remains now to identify which of the equations is valid in the pre-gelation stage and which is valid post-gelation. We know that prior to the occurrence of gelation in the coagulating system, the total mass of the solution is given by

$$M_1(t) = M_1(0) + \int_0^t \int_0^\infty \lambda\, g(\lambda, s)\, d\lambda\, ds, \qquad \text{for } t \in [0, T_{gel}) \tag{4.303}$$

In terms of differential equations, the above reads

$$M_1'(t) = \int_0^\infty \lambda\, g(\lambda, t)\, d\lambda \qquad \text{for } t \in [0, T_{gel}) \tag{4.304}$$

$$\text{subject to I.C. } M_1(0) = \int_0^\infty \lambda\, c_0(\lambda)\, d\lambda = \frac{k}{m}\,(\sigma - \sqrt{\sigma^2 - m^2}). \tag{4.305}$$

Furthermore, after the gelation has occurred it is expected that the equality no longer holds and we have

$$M_1(t) < M_1(0) + \int_0^t \int_0^\infty \lambda\, g(\lambda, s)\, d\lambda\, ds, \qquad \text{for } t \geq T_{gel}. \tag{4.306}$$

(see e.g. [15]). Based on these relations we decide next on the corresponding equations (4.301) and (4.302) for $v(t)$ in the pre- and post- gelation stages.

Claim 4.1 *The differential equation (4.301) corresponds to the pre-gelation regime.*

Proof. Indeed, since $v'(t) = Q'(t) = M_1(t)$ and $v''(t) = M_1'(t)$ then using the form of the function $\varphi(t) = k\,t + m$, the ODE (4.301) becomes

$$v''(t) = \frac{k}{k\,t + m}\, v'(t)$$

which reduces to an I.V.P. for $M_1(t)$:

$$M_1'(t) = \frac{k}{k\,t + m}\, M_1(t), \quad \text{subject to} \quad M_1(0) = \frac{k}{m}\,(\sigma - \sqrt{\sigma^2 - m^2}).$$

Integrating the above w.r.t from 0 to t we obtain the following equality

$$M_1(t) = M_1(0) + \int_0^t \frac{k}{k\tau + m}\, M_1(\tau)\, d\tau. \tag{4.307}$$

More explicitly, $M_1(t) = \frac{k}{m^2}\,(\sigma - \sqrt{\sigma^2 - m^2})\,(kt + m)$. On the other hand, if we rewrite the source function $g(\lambda, t)$ in terms of known functions $\varphi(t)$ and $c(\lambda, t)$ then we have

$$g(\lambda, t) = \frac{k\, e^{R(t)}}{m\, S(t)}\, c(\lambda, t)$$

and using the definitions of $S(t)$, $R(t)$ and since $A_2 = a = 1$ then we obtain

$$S(t) = P(t) = \frac{\varphi^2(t)}{m^2} \quad \Rightarrow \quad e^{R(t)} = [P(t)]^{1/2} = \sqrt{S(t)} = \frac{\varphi(t)}{m} \quad \text{and} \quad \frac{e^{R(t)}}{S(t)} = \frac{m}{\varphi(t)}.$$

Therefore, we obtain $R(t) = \ln\left(\frac{k\,t+m}{m}\right)$. Substituting everything into $g(\lambda, t)$, we obtain

$$g(\lambda,t) = \frac{k}{\varphi(t)}\,c(\lambda,t) \quad \Rightarrow \quad \int_0^t\int_0^\infty \lambda\, g(\lambda,\tau)\,d\lambda\,d\tau = \int_0^t \frac{k}{k\,\tau+m}\,M_1(\tau)\,d\tau. \quad (4.308)$$

Combining (4.307) with (4.308) then (4.303) holds which makes (4.301) hold for the pre-gelation stage (still T_{gel} is unknown) and thus the claim is proved.

Now, it remains to show that the other DE (4.302) corresponds to the post-gelation regime ($t \geq T_{gel}$), that is we need to show (4.306) is a result of (4.302). In order to solve the DE (4.302) we need to know the gelation time T_{gel} since the initial condition for (4.302) is considered as $v(T_{gel})$, where v is the solution to (4.301). As is the case [34, 70], the gel-time is determined as the first instance when the second moment of solution $M_2(t) = u_x(0,t)$ blows up to infinity. This corresponds to the time when $v(t) = \varphi(t)$, where $v(t)$ is the solution of (4.301). First, let's calculate the expression of $v(t)$ in (4.301). We have

$$v'(t) = M_1(t) = \frac{k}{m^2}\,(\sigma-\sigma_0)\,(kt+m)$$

subject to the I.C. $v(0) = \sigma$, where $\sigma_0 = \sqrt{\sigma^2 - m^2}$, with $\sigma \geq m > 0$. We obtain

$$v(t) = \sigma + \frac{k}{m^2}\,(\sigma-\sigma_0)\left(\frac{k}{2}\,t^2 + m\,t\right) \quad \text{for} \quad t \in [0, T_{gel}) \qquad (4.309)$$

Or,

$$Q(t) = \frac{k}{m^2}\,(\sigma-\sigma_0)\left(\frac{k}{2}\,t^2 + m\,t\right).$$

To determine T_{gel} we need to solve the quadratic equation in t. Using the definition of σ_0 above we obtain

$$\sigma + \frac{k}{m^2}\,(\sigma-\sigma_0)\left(\frac{k}{2}\,t^2 + m\,t\right) = k\,t+m \quad \Rightarrow \quad t - \frac{m}{k}\left(\sqrt{\frac{\sigma+\sigma_0}{\sigma-\sigma_0}} - 1\right) = 0.$$

Therefore, the gel-time is given by

$$T_{gel} = \frac{m}{k}\left(\sqrt{\frac{\sigma+\sigma_0}{\sigma-\sigma_0}} - 1\right) =: T_{gel}(g>0). \qquad (4.310)$$

In the post-gelation regime ($t \geq T_{gel}$), the unique solution $v(t)$ to the equation (4.299) is given by $v(t) = \varphi(t) = k\,t+m$. Such an assertion holds indeed true since it is clear that such a function satisfies the ODE (4.299) and the I.C. $v(T_{gel}) = v(t)|_{t=T_{gel}}$

where $v(t)$ is the solution obtained in (4.309). Hence, the expression of $v(t)$ for $t \geq T_{gel}$ is given by $v(t) = k\,t + m$. Then, $v'(t) = M_1(t) = k$, so $M_1(t) = k =$ constant and $Q'(t) = M_1(t) = k$.

Alternatively, to show that $v(t) = k\,t + m$ is indeed the post-gelation solution to (4.299) or $M_1(t) = k$ for $t \geq T_{gel}$ then we return to the inequality (4.306), for $t \geq T_{gel}$ and see that this holds true.

Comparing the gel-time in (4.310) to the gel-time $T_{gel}(g = 0) := \frac{m}{k} \frac{\sigma_0}{\sigma - \sigma_0}$ that we obtained in Example 4.14, for the sourceless case we obtain as expected that $T_{gel}(g > 0) \leq T_{gel}(g = 0)$, as $\sigma \geq m$, i.e. that the gel-time in the presence of source terms occurs sooner than in the absence of source terms (as was proved in general for the kernels $K(\lambda, \mu) = \lambda\,\mu$ in [15]). Thus, we have obtained the formula for $Q(t)$ in the particular case of Example 4.16, and thus our example is completely proved.

Some remarks for the general coagulation kernel $K(\lambda, \mu)$

Prior to studying the application of the symmetry group methods to the modified coagulation equation (4.176) we also applied the group method successfully to the coagulation equation (4.169) with both nonlocal terms: the convolution and the infinite integrals. For a general coagulation kernel $K(\lambda, \mu)$, where the coagulation equation cannot be modified to obtain (4.176), and assuming that there are no particle source terms in the system, the generators of the Lie group of point transformations admitted by (4.169) are given by $\xi_1(\lambda) = 0$, $\xi_3(t) = -c_1\,t + c_2$, $\eta_1(f) = c_1\,f$, where c_1, c_2, are arbitrary constants. In this case, solving the invariant surface condition (4.45), we have obtained the similarity variable and similarity solution to be given as

$$s \equiv \lambda = \text{constant} \quad \text{and} \quad c(\lambda, t) = \psi(\lambda)\left(t - \frac{c_2}{c_1}\right)^{-1}$$

where the similarity profile $\psi(\lambda)$ satisfies the IDE

$$\psi(\lambda) = -\frac{1}{2}\int_0^{\lambda} K(\lambda - \mu, \mu)\,\psi(\lambda - \mu)\,\psi(\mu)\,d\mu + \psi(\lambda)\int_0^{\infty} K(\lambda, \mu)\,\psi(\mu)\,d\mu \quad (4.311)$$

In general, (4.311) cannot be solved analytically, and numerical methods need to be employed. We leave this as future work.

Remark 4.15 *Solutions of the form* $\frac{\psi(\lambda)}{t+c}$, *where c is an arbitrary constant, are constructed by da Costa [21] and Leyvraz [64] for the discrete coagulation equation. These solutions were actually the first examples of gelling solutions for kernels of the form* $K_{i,j} = i^{\alpha}\,j^{\beta} + i^{\beta}\,j^{\alpha}$, *where* $1 < \alpha + \beta < 2$.

Chapter 5

Numerical methods for coagulation equations

5.1 Review of previous work

In this section we present a brief summary of a family of deterministic numerical methods existing in the literature for solving the coagulation equation

$$\frac{\partial c}{\partial t}(x,t) = \frac{1}{2}\int_0^x K(x-y,y)c(x-y,t)c(y,t)\,dy - c(x,t)\int_0^\infty K(x,y)c(y,t)\,dy + g(x,t) \tag{5.1}$$

The exact evolution of the size distribution $c(x,t)$ depends on the nature of the collision kernel, the amount of inclusion/removal of particles and the initial size distribution. Analytical solutions to the coagulation equation (5.1) have only been found for a few forms of $K(x,y)$ and $g(x,t)$, including the forms in Chapter 4.

In situations of practical interest, the functional forms of K and g are such that (5.1) must be solved numerically. Due to the computational difficulties in solving (5.1), only a few numerical solutions have been reported in which both coagulation processes with sources and sinks are included. Analytical solutions are available for certain special cases of equation (5.1). Three major approaches are used to represent the size distribution of aerosols: continuous, discrete and parametrized. In this thesis we focus only on the numerical approximations of continuous models, that is both the size distributions and coagulation equations are in continuous form.

During the last century, several numerical methods (algorithms) have been proposed to solve the coagulation equation (5.1). The first term is of nonlinear Volterra type in the language of integral equations. The difficulty of solving accurately such an integro-differential equation is due to the fact that the limit of integration in the convolution integral depends on the size variable x and the integrands are quadratic functions. On the other hand, the infinite integral which depends on the size distribution function seems to create difficulties, especially if one truncates the domain to a finite range.

In the open literature, several numerical methods have been developed for solving the coagulation equations. These methods include: the method of moments, finite element methods and weighted residual methods, orthogonal collocation method over finite elements, discretized population balances, finite difference methods, mesh techniques, finite volume methods, power series solutions, etc. Surveys of several popular numerical methods for particulate dynamic equations are given in [25, 59, 88, 113]. In the following we present briefly some of the deterministic methods that have been developed in the literature for population balance equations (PBEs) that include the coagulation equation as a particular case.

5.1.1 Method of moments

The method of moments is one of the oldest and most widespread methods for solving the coagulation equation. This method works by representing the equation in terms of the size distribution moments. The moment method tracks the time dependence of the lower order radial moments of the distribution defined as $\mu_k = \int r^k f(r)\, dr$, where the index k refers to the k^{th} moment and $f(r)$ is the size distribution function. The basic idea behind this method is that the coagulation equation is transformed into a closed set of ordinary differential equations that provide the exact solution for the moments [9, 78]. The conventional formulation of the moment method requires that the moment evolution equations involve only functions of the moments themselves. This requirement significantly restricts the application of the method to aerosol-related problems, since only for very few special cases of coagulation kernels one can reduce (5.1) to a closed form equation for the moments. In the method of moments, the particle size distribution is not tracked directly but through its moments. Previous studies have shown that the accuracy and computational time depend largely on the relative magnitude of the moments - one then needs to modify the moments in a controlled manner. In addition, solution of differential equations for the moments requires excessive computational resources.

5.1.2 Finite element methods and methods of weighted residuals

These methods retrieve the size distribution by approximating the solution as a linear combination of basis functions over a finite number of subdomains, also called "elements", whose coefficients are to be determined so that their sum satisfy the coagulation equation. Weighted residual methods with global functions were among the first to be tried in the early work of Ramkrishna [87].

The earliest notable attempt to solve the coagulation equation with FEMs was provided by Gelbard and Seinfeld [48] in 1978, who considered both orthogonal collocation on finite elements and spline collocation for the solution of the PBEs that include coagulation equation (5.1). In their article, the semi-infinite particle size domain is truncated at some large value and then scaled logarithmically. Furthermore, the finite domain is divided into elements, to avoid ill-conditioning systems. The authors evaluate the "finite-domain error", i.e. the error incurred by the solution on a finite domain $[v_a, v_b]$, where the lower and upper limits v_a and v_b on the volume are selected such that

$$M_i(t) = \int_{v_a}^{v_b} x^i\, c(x,t)\, dx \Big/ \int_0^\infty x^i\, c(x,t)\, dx, \quad \text{for} \quad i = 0, 1$$

do not differ appreciably from unity. The authors notice from their experiments that in the case of a constant and linear kernel K, the deviation between the numerical and exact solutions increases with time - the numerical solution lies above the exact one. This is due to the fact that the numerical solution does not account for collisions between particles inside the computational domain $[v_a, v_b]$ with those particles of sizes larger than v_b. The authors suggest that the finite domain errors can be significantly reduced by the presence of removal mechanisms which serve to reduce the number of particles at the large end of the spectrum (see e.g. [48, 85]).

The method proposed in [48, 85] was later applied to solve the population balance equation (see Erasmus et al [33]) and the Lifshitz-Slyozov equation of continuity (see Eyre [40]). Their approach is based on a projection method with cubic B-splines (as basis functions) where Galerkin and collocation techniques were used to determine the spline coefficients. In their formulation, the authors scaled the domain with a singular function by using a change of variable which maps the infinite domain for the particle size onto $[-1, 1]$ such as $x \in [0, \infty) \mapsto \zeta\left(\frac{1+v}{1-v}\right) \in [-1, 1]$. However, it seems more difficult to control the distribution of mesh points [41]. Moreover, the methods provided by Erasmus et al [33] and Eyre [40] rely upon well-chosen mapping parameters. The authors acknowledge that a good choice of their mapping parameter ζ (selection being made by trial and error) contribute to the success of their methods. In a recent work, Sandu et al [93] generalize the work of Seinfeld et al [48] to splines of arbitrary orders. A general framework for the discretization of particle dynamics equations has been proposed recently by Sandu et al [90] by using projection methods, which include Galerkin and collocation techniques. Test problems include very small constant coefficients of the form $K(x, y) = 2.166 \times 10^{-6}$. The methods proposed by Sandu et al [90] are not conservative, i.e. they do not exactly conserve the total particle number and volume. Also they are not positive definite, i.e. they do not guarantee a nonnegative numerical distribution. One of the main disadvantages of this framework is the computational expense associated with some of the tensors corresponding to the coagulation integrals.

5.1.3 Discretized population balances (DPBs)

These methods emerged as the main alternative to FEMs: they are esentially finite difference schemes. These methods consist of discretizing the particle-size domain into intervals and assuming the particle size distribution function be constant within each of these intervals. In the classical formulation of these methods, the integrals are replaced with summations. The DPBs differ in their choice of discretization (linear, geometric, arbitrary) and the assumption about the shape of the size distribution within each interval [67]. Hounslow et al [78] have used and developed a geometric discretization of the size domain $x_{i+1}/x_i = 2$ which correctly predicts the rate of change of total number of particles and volume. However, for higher particle size distributions a much finer grid (discretization) is needed. This could be achieved by using an adjustable geometric size discretization of the form $x_{i+1}/x_i = 2^{1/q}$, where q is an integer larger than 1, as proposed by Litster et al [67]. The latter technique allows for a precise prediction of higher moments and the shape of the particle size distribution. Hounslow et al [78] show that some of the DPBs yield significant errors in the prediction of the total number or total volume of particles. In general, the most accurate DPBs are the most tedious to solve numerically, with many integration within each size interval. As pointed out by Gelbard et al [48], these methods lead to severe errors unless a uniform grid is employed, which is only valid for systems that exhibit very small size ranges. However, for such processes such as coagulation of aerosols, where very large particles are created rapidly through aggregation, a nonuniform exponential grid must be employed (see [67, 78]). Kumar and Ramkrishna [59] reviewed the previous methods, and observed that uniform discretization in volume (size) gives good accurate results but requires a large number of classes (sections) to cover the whole size range. They proposed a generalized method that preserves two arbitrary particle size distribution properties (such as the moments) while relaxing other properties. This fixed pivot technique uses a geometric grid of the form $x_{i+1} = s\,x_i$. For example, for the pure coagulation equation with $K(x, y) = x\,y$: for moderate sizes a course grid with $s = 1.5$ provides accurate solutions, whereas for larger sizes a finer grid with $s = 1.15$ is required. This leads to an improvement in accuracy and reduced computational effort. Kumar et al [60] also presented a moving pivot method which takes into account the variation of the number density within each size range. This method gives extremely accurate results.

A comparison of the methods in **5.1.2** and **5.1.3**, shows that due to the excessive computational demands and the complexity of the implementation raised by the FEMs and other function approximation methods, the DPBs seem to attract more and more attention, especially when applied to the population balance equations (see the recent work of Rigopoulos and Jones [88]).

5.1.4 Finite difference methods

Krivitsky in [58] obtained the numerical solution to the pure coagulation equation (5.1) for two types of coagulation kernels $K(x, y) \approx (x + y)^{\lambda}$ and $K(x, y) \approx (x\,y)^{\lambda/2}$, where $0 < \lambda \leq 2$. The author introduced a finite limit size M up to which computations were executed (physically corresponding to a sink of particles at large sizes). The collision integral on the right-hand side was computed by the trapezoidal formula, using a linear interpolation, while the second integral was truncated to the finite value M and then approximated by the trapezoidal rule. The resulting differential equation was solved by using a second-order Runge-Kutta method. It was found that for rapidly growing kernels, at some time a small distortion appeared in the plot of the distribution function, which grows rapidly after a short time. To make the procedure stable, it is necessary to take a very small stepsize Δt at the expense of increasing the parameter M. The author investigated the cases when the gelation phenomenon is present and the influence of a finite M on the solution. The numerical experiments show that the total mass begins to decrease earlier than the gel-time T_{gel}; also there is a rise on the right-end of the distribution function at $x \approx M$ for t larger than the gel-time T_{gel}.

5.1.5 Finite volume methods

Filbet and Laurençot [41] developed a numerical scheme for the pure coagulation equation which relies on a conservative formulation and a finite volume approach. In their paper, the authors truncate the volume variable to some maximal value R, and choose a nonconservative approximation of the coagulation term that is suitable for reproducing the gelation phenomenon. Using explicit available solutions to test the accuracy of the numerical scheme, it has been observed that for rapidly increasing coagulation coefficients K a larger truncation parameter R has to be chosen as these kernels yield a faster transfer of matter towards larger and larger volumes. For kernels such as $K(x,y) = x\,y$ the truncation of the particle domain seems to greatly influence the large size behaviour after the numerical gelation time. Also, a decrease of the moments has been observed after the gel-time. In these cases, a much larger truncation parameter R is needed and thus computationally the cost and the numerical error are both increased.

5.1.6 Power series methods

Melzak [74], was the first to provide theoretical results through the technique of power series expansion in the time variable. Melzak approximated the solution of the pure coagulation equation by means of a power series of the form $c(x,t) = \sum_{i=0}^{\infty} a_i(x)\,t^i$. However, a few problems arise when one attempts to use this type of series, such as: the amount of computation becomes prohibitive very rapidly as i increases in value; many terms are needed in the series to give a good approximation for $c(x,t)$ at large values of x; the interval of convergence for the series is very small. Martynov et al [71] suggested that the finite interval of convergence of such series can be eliminated by a change of time variable in the system of the form: $T = 1 - M_0(t)/M_0(0)$ and a series of the form $u(x,T) = \sum_{i=0}^{\infty} a_i(x)\,T^i$ can be used. However, the authors soon understood that the use of such a series is only practical for the initial stages of the evolving spectrum under arbitrary initial conditions and with variable kernel $K(x,y)$.

Conclusion

Most of the numerical work proposed in the literature of coagulation equations applies to the case when no particle sources and sinks are present in the system since only in these cases analytic solutions are known. Moreover, all the deterministic numerical methods presented above are able to accurately predict the size distribution function for cases where the rate of coagulation $K(x, y)$ is either constant or linear in the variables x and y. For gelling-type kernels $K(x, y) = x\,y$ with $g \equiv 0$, these methods provide qualitative agreement between the numerical and analytical solutions only for a small period of time. The methods developed by Kumar et al [59, 60] is one of the first methods that provides good estimates for the solution of the pure coagulation. However, as pointed out earlier, these methods rely on the fact that the discrete equations for aggregation processes be internally consistent (preservation of two properties of the distribution) with regard to some specific moments of the size distribution. Even though such a method brings an improvement over other previous numerical methods its applicability to more general kernels K is limited.

In the next two sections of this chapter we provide a few numerical (improved) approaches to obtain accurate numerical approximations to the solution of the coagulation equation with particle source terms. To validate our numerical work we compare the numerical solutions using the explicit available solutions ($g(x, t) = 0$) to (5.1) obtained in the literature, or our new similarity (group invariant) solutions provided in Sections 4.2 and 4.3 for $g(x, t) \geq 0$.

5.2 Bounded coagulation kernels

In this section, we present two reliable numerical methods to solve the coagulation equation for a class of bounded coagulation kernels with particle source terms

$$\frac{\partial c}{\partial t}(x,t) = \frac{1}{2}\int_0^x K(x-y,y)c(x-y,t)c(y,t)\,dy - c(x,t)\int_0^\infty K(x,y)c(y,t)\,dy + g(x,t) \tag{5.2}$$

subject to the initial condition

$$c(x,0) = c_0(x). \tag{5.3}$$

Quite a few numerical schemes were investigated, and the two methods yielding the most accurate results (when tested in cases where exact solutions are known) were found to be the weighted residual method (collocation method) and the method of adaptive power series at successive points. Using these methods we investigate the dynamic behaviour of the size distribution c for some choices of the problem parameters (initial condition c_0, coagulation coefficient K and source term g). In addition, we analyze the dependence of the solution on these parameters.

One of the issues we address in this section regards the computation of the values of $c(x,t)$ for a bounded, pre-determined range of values $0 \leq x \leq X$ and $0 \leq t \leq T$. This is the correct setting in many industrial problems, where the physical limits X on the particle size and T on the reaction time arise naturally. In such cases we may, if desired, find constants m, n, p such that the change of variables

$$x = mx^*, \qquad t = nt^*, \qquad c = pc^*,$$

transforms (5.2) into an analogous equation with the same K, but with $0 \leq x^*$, $t^* \leq 1$ (or any other finite upper limits; the modification is in c_0 and g being multiplied by various constants). In other words, in this type of problem it is legitimate to confine x and t to a pre-determined range of values.

The other problem (which we shall not discuss here) typically involves a change of variables $t^* = \psi(t)$, the function ψ being chosen in such a way that the entire interval $0 \leq t < \infty$ corresponds to $0 \leq t^* < 1$; a popular choice is $t^* = \left[\int_0^\infty (c_0(x) - c(x,t))dx\right] / \left[\int_0^\infty c_0(x)\,dx\right]$. This is most suitable for studying the long-time properties of $c(x,t)$, since $t \to \infty$ corresponds to $t^* \to 1^-$. The method, however, appears to be less reliable numerically for bounded ranges of the values of t (see e.g. [25, 71]).

5.2.1 Adaptive power series method (APS) at successive points

One of the more reliable methods of obtaining numerical solutions to (5.2) especially for coagulation kernels K that are bounded functions of x and y, turns out to be the use of adaptive power series. If K is independent of time, then we can approximate both the solution and the source term by power series of the form

$$c(x,t) = \sum_{i=0}^{\infty} \gamma_i(x)\, t^i \quad \text{and} \quad g(x,t) = \sum_{i=0}^{\infty} \delta_i(x)\, t^i$$

for some interval of values of x and t. If we substitute c and g above into (5.2) and equate like powers of t, then the following recursion formula for the coefficients $\gamma_n(x)$ can be derived:

$$\gamma_0(x) = c_0(x)$$

and

$$\begin{aligned}(n+1)\gamma_{n+1}(x) = \delta_n(x) &+ \frac{1}{2}\sum_{i+j=n}\int_0^x K(y, x-y)\,\gamma_i(y)\,\gamma_j(x-y)\,dy \\ &- \sum_{i+j=n}\gamma_i(x)\int_0^\infty K(x,y)\,\gamma_j(y)\,dy, \quad \text{for} \quad n \geq 0. \end{aligned} \tag{5.4}$$

Melzak [74] was the first to prove theoretical results (global existence and uniqueness of solutions) for the pure coagulation equation ($g \equiv 0$) using the technique of power series expansion in the time variable t (see e.g. [25, 74]). The question of the convergence of the series $\sum_{i=0}^{\infty} \gamma_i(x)\, t^i$ is a very interesting one, not least because there is more than one sense in which the series can converge. The question of convergence and an example of its use will be discussed in a future work, see e.g. Calin et al [16].

In principle, given the coagulation kernel K, the initial size distribution c_0 and the source term g, one can evaluate the coefficients γ_n one by one and obtain the exact solution of (5.2). However, solving the nonlinear, many-term recursion formula in (5.4) for the general term γ_n is not straightforward. Moreover, the integrals in (5.4) can only be evaluated in closed form for very special cases of K, c_0 and g; in general, numerical integration needs to be employed. Hence, one can attempt to make use of truncated power series approximations for $c(x,t)$ and $g(x,t)$. However, even with a truncated power series, as n increases the amount of computation becomes burdensome. This is due to the fact that many terms are needed in the series in order to obtain a good approximation for $c(x,t)$ at large values of x.

For additional comments on the method of power series expansions in terms of the small parameter $t^* = \psi(t)$, see Martynov et al [71]. They comment that, for certain kernels, using 10 terms in the series yields reasonable results only for $t^* x \leq 2$. This is only practical for the initial stages of the evolving spectrum. Drake [25] suggests the use of power series combined with asymptotic methods for obtaining global numerical solutions.

Our proposed numerical method (APS) is as follows: In using a partial sum

$$c(x,t) \sim \sum_{i=0}^{m} \gamma_i(x) t^i$$

for relatively large times t, a modification is found to be useful: Let $\delta > 0$ be small, and suppose we want to find the value of $c(x,t)$ at $t = n\,\delta$ for some large n. For this reason, we start with $\gamma_0 = c_0$ and compute $\gamma_1, \ldots, \gamma_m$ using the recursion formula (5.4). For the approximation of these integrals the trapezoidal rule yields the most accurate results. However, for the approximation of the second integrals in (5.4) we use Simpson's rule. Thus, we obtain $c(x,\delta) \sim c^{(1)}(x) = \sum_{i=0}^{m} \gamma_i(x)\delta^i$. However, to compute $c(x, 2\delta)$, it is better to start with a new $\gamma_0^{(2)} = c^{(1)}$, re-compute the corresponding $\gamma_1^{(2)}, \ldots, \gamma_m^{(2)}$ from (5.4), and then use

$$c(x, 2\delta) \sim c^{(2)}(x) = \sum_{i=0}^{m} \gamma_i^{(2)}(x)\delta^i.$$

This is tantamount to computing the Taylor series at $t = \delta$, which is in turn equivalent to shifting the origin of time to $t = \delta$, and then solving the initial-value problem. Proceeding in this way, we have found that the numerical results are much more precise than when a single series $\sum_{i=0}^{m} \gamma_i(x) t^i$ was used for increasingly larger values of t.

For numerical purposes, to approximate (5.4) and thus (5.2) we consider a uniform grid $x_k = (k-1)\,\Delta x$, where $\Delta x = \frac{X}{N-1}$, for $k = 1, \ldots, N$. First, we impose that the equation (5.4) holds exactly at the node points x_k (collocation points). Based on the description above, we calculate the discretized numerical solution $c^h(x_k, t)$ at a large time $t = n\,\delta$. In the framework of purely discrete populations and uniform grid, the size of a new aggregate always matches exactly with the size of one of the x_i's. Therefore, a uniform grid allows us to avoid the use of an interpolation technique, which otherwise would be needed especially to deal with the approximation of the convolution integral in (5.4), even with a trapezoidal rule.

5.2.2 Collocation method

To validate the results of our numerical scheme (using APS method) in cases where no exact solutions are known, we have also implemented the collocation method suggested by Sandu et al [90], with slight modifications.

To solve numerically the equation (5.2) using the collocation method, we first discretize the particle size domain $[0, X]$ in a finite number N of size bins (increments in space) of the form $B_k = [x_k, x_{k+1}]$, for $k = 1, 2, \ldots, N-1$, with $x_1 = 0$ and $x_N = X$, and same width Δx as in Section 5.2.1. As is generally the case with the weighted residual method, the approximated size distribution function $c(x, t)$ is searched for in the form of a finite-dimensional approximation:

$$c^h(x,t) = \sum_{i=1}^{N} c_i(t)\, \phi_i(x),$$

where $\{\phi_1(x), \ldots, \phi_N(x)\}$ is a set of continuous functions called basis (or trial) functions. This approximation is substituted into (5.2). Next, we multiply the residual equation by a test function $\xi_j(x)$, for $j = 1, 2, \ldots, N$ and integrate over the domain $[0, X]$ to obtain a variational (weak) formulation. In the collocation framework, the test functions are chosen as delta Dirac functions at special points, called collocation points. In our study case, we choose the collocation points as the node points. Thus, the test functions are given as follows $\xi_j(x) = \delta(x - x_j)$. The advantage of using node points is that the "mass" matrix becomes the unit matrix $I_{N\times N}$ which helps minimizing the computational cost. In addition, we choose as basis functions the piecewise polynomial functions

$$\phi_i(x) = \begin{cases} \frac{x - x_{i-1}}{\Delta x}, & \text{if } x_{i-1} \le x \le x_i, \\ \frac{x_{i+1} - x}{\Delta x}, & \text{if } x_i \le x \le x_{i+1}, \\ 0, & \text{otherwise} \end{cases}$$

for $i = 1, 2, \ldots, N$. These basis functions are piecewise continuous linear functions that satisfy $\phi_i(x_j) = 1$, if $i = j$ and 0, if $i \ne j$, which in addition have a compact support. The latter property for the basis functions ϕ_i, helps us simplify the calculations for the coagulation tensors (which we denote by I_1 and I_2) since only the nonzero entries are computed. For the computation of the coagulation tensors we use a 3-point and 2-point Gaussian numerical quadrature, respectively. Having performed the pointwise evaluation of the coagulation terms at the nodal points, the original coagulation equation (5.2) is transformed into a set of nonlinear ordinary differential equations, where the dependent variables are the coefficients $c(t) = [c_1(t), \ldots, c_N(t)]^T$, see [90]:

$$c'(t) = [(I_1 - I_2) \times c(t)]\, c(t) + g(t) \tag{5.5}$$

where $g(t) = [g_1(t), \ldots, g_N(t)]^T$, with $c_i(t) = c(x_i, t)$ and $g_i(t) = g(x_i, t)$, for $i = 1, 2 \ldots, N$. Our experiments showed excellent accuracy even with piecewise-linear elements and with a small number N of size bins.

The use of collocation methods over Galerkin methods is preferred since it does not require extensive integral evaluations, and thus it leads to considerable computational savings. For a complete theoretical description of the projection methods (including Galerkin and collocation methods) see e.g. Atkinson [5].

5.2.3 Some numerical experiments

Our numerical results are presented for $0 \leq x \leq 5$ and $0 \leq t \leq 1$ following the comments at the beginning of Section 5.2. Even though the collocation method requires integration only at the nodal points and seems to have good accuracy even with linear elements, computationally speaking it is an expensive method. For instance, if we choose the parameters $g \equiv 0$, $K \equiv 1$ and $c(x, 0) = \exp(-x)$ then using 31 bins yields a maximum error of 1.67×10^{-3} with the collocation method, and a maximum error of 1.72×10^{-3} for the adaptive power series method (with terms up to and including t^2). Moreover, the errors were found to be of a similar order of magnitude in other examples we looked at. Our conclusion from repeated testing is that, for examining the *qualitative behaviour* of the solutions, the adaptive power series is quite accurate even with as few as three terms. For more precise numerical solutions the collocation method is preferred.

Our first two examples consider the coagulation equation with a constant kernel $K \equiv 1$, an initial distribution $c(x, 0) = \exp(-x)$ and two cases of source terms $g(x, t) = 0$ and $g(x, t) = T(t)^2 \exp(t - x\,T(t))$, where $T(t) = 2/(1 + \exp(t))$. In this case, the corresponding exact solutions are $c(x, t) = (1 + t/2)^{-2} e^{-2x/(2+t)}$ and $c(x, t) = T^2(t) \exp(t - x\,R(t))$, respectively. Both solutions have been obtained using Example 4.15 (with $R(t) = 0$ and $R(t) = t$ in the notation of that example). Our numerical results show that both the adapted power series and collocation methods accurately predict the numerical solution $c^h(x, t)$. For our purposes we have sketched the approximation c^h (using both methods) and the analytical solution c at a fixed time as shown in Figures 5.1, 5.2).

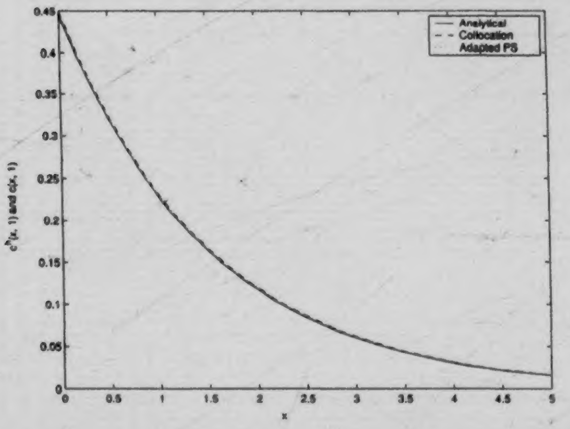

Figure 5.1: Plot of the numerical solution $c^h(x,1)$ for $g \equiv 0$, using the collocation and the adaptive power series methods and analytical solution $c(x,1)$.

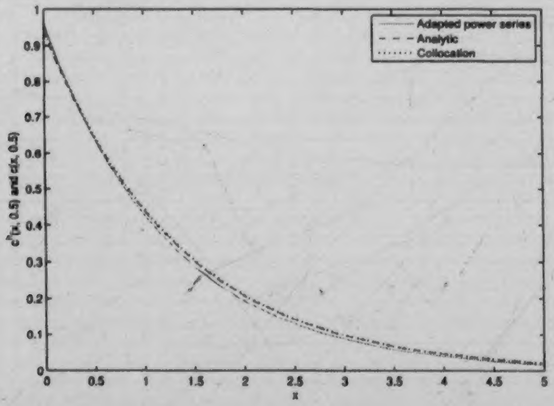

Figure 5.2: Plot of the numerical solution $c^h(x,0.5)$ for $g > 0$, using the collocation and the adaptive power series methods and analytical solution $c(x,0.5)$.

Next, we consider a few examples of kernels K for which no analytical solutions are known. The adaptive power series method is used in the next examples and subsequent graphs. Longer time periods can be investigated by a suitable change of variables as indicated earlier in this section, but result in no qualitative change in behaviour.

Figure 5.3 shows the propagation of an initial global maximum $c(x,0) = e^{-(x-1)^2}$ through time.

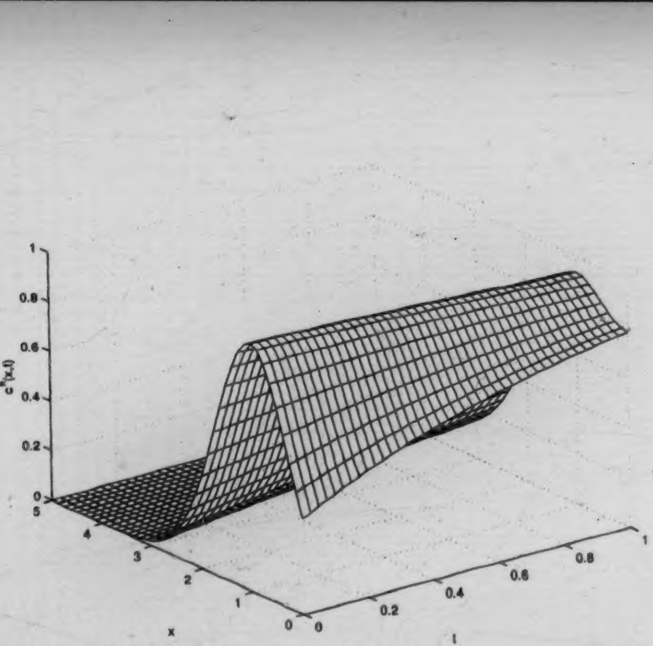

Figure 5.3: $K(x,y) = 1/(1+x+y), \quad g(x,t) = e^{-x}, \quad c(x,0) = e^{-(x-1)^2}$.

Similarly, if the initial condition has two maxima, as in Figure 5.4, then the same feature appears to persist in the solution for all time. Figure 5.4 shows the solution $c^h(x,t)$ at various times $t = 0, 0.25, 0.5, 0.75, 1$.

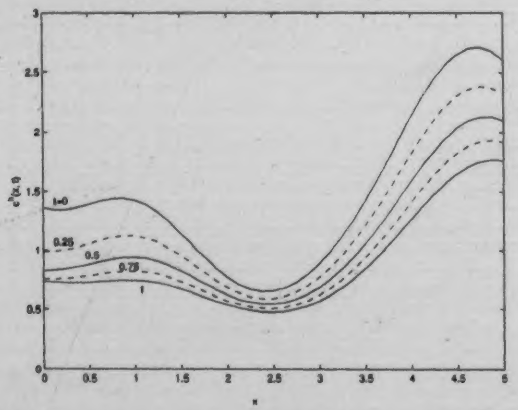

Figure 5.4: $c(x,0) = e^{-\sin x} + e^{-(x-1)^2}$, $K(x,y) = 1/(1+x+y), \quad g(x,t) = e^{-x}$.

The graph in Figure 5.5 shows the influence of the source term on the solution. The solution increases from its initial value of $c_0(x) = 0$. The series of graphs in Figure 5.5 also indicates the fact that the kernel K exerts a relatively small and transient influence on the form of the solutions, with the initial conditions c_0 and the source term g being the more dominant factors.

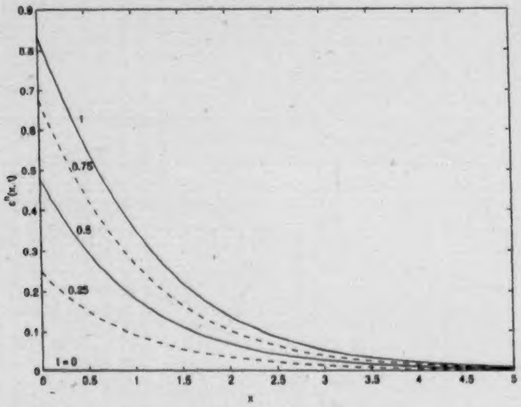

Figure 5.5: $K(x,y) = 1/(1+x+y), \quad g(x,t) = e^{-x}, \quad c(x,0) = 0.$

Our last example in this section (Figure 5.6) is that of another intractable kernel, $K(x,y) = e^{-(x^2+y^2-1)^2} = e^{-(r^2-1)^2}$ (in polar coordinates). Here we observe that the maxima of K initially appearing in the solution is being smoothed out by the coagulation process.

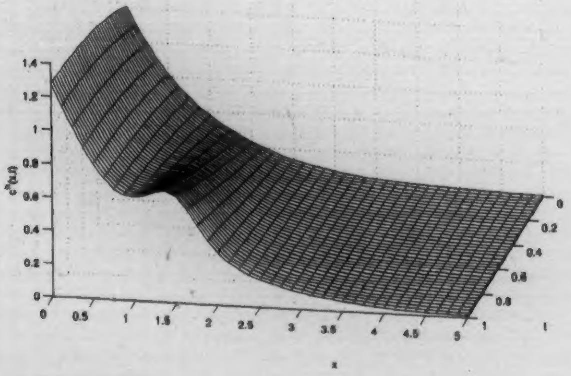

Figure 5.6: $K(x,y) = e^{-(x^2+y^2-1)^2}, \quad g(x,t) = e^{-x}, \quad c(x,0) = e^{-x}$

5.3 Unbounded coagulation kernels

Although there have been many attempts in the literature to solve the coagulation equation numerically, there still is not a good, accurate numerical method that deals with bilinear, separable kernels of the form $K(x,y) = (\alpha+\beta\, x)(\alpha+\beta\, y)$, where $\alpha \geq 0$ and $\beta > 0$ are some arbitrary constants, in the presence of particle sources. Our main purpose in this section is to provide some numerical results for unbounded kernels of the form above in the absence and presence of particle source terms. The method that we provide is based on a direct discretization of (5.2), followed by quadrature methods for the integral terms (based on Trapezoidal, Simpson and Gauss-Laguerre quadrature) and time-integration of the system of ODEs. A uniform grid was used for numerical discretization. To test our numerical results we compare the numerical solutions with corresponding solutions obtained by collocation methods (Section 5.2.2) and also explicit solutions obtained in Sections 4.2 and 4.3.

As described in the review of numerical methods in Section 5.1, when solving the coagulation equation numerically, the first step is to reduce the theoretical infinite domain for the size variable x to a finite range $0 = X_{min} \leq x \leq X_{max}$. This constraint comes from a physical limit X_{max} in many industrial problems. Based on the form of the coagulation kernel K at the beginning of this section, it seems more natural to provide the numerical method for the function $n(x,t) = \theta(x)\, c(x,t)$. For this purpose, we multiply the equation (5.2) by $\theta(x)$ to obtain the new form of the coagulation equation

$$\frac{\partial n}{\partial t}(x,t) = \frac{\theta(x)}{2}\int_0^x n(x-y,t)n(y,t)\,dy - \theta(x)\,n(x,t)\int_0^\infty n(y,t)\,dy + \theta(x)\,g(x,t) \tag{5.6}$$

subject to the initial condition

$$n(x,0) = n_0(x) = \theta(x)\,c_0(x) = (\alpha+\beta\, x)\,c_0(x). \tag{5.7}$$

5.3.1 The numerical method

After we have reduced the computational domain to a finite interval, the next step in solving equation (5.6) numerically is to introduce the size and time discretization. For this purpose, we choose a mesh of $[0, X_{max}]$ to be a uniform grid x_i, $0 \leq i \leq N_x$ with spacing $\Delta x = \frac{X_{max}}{N_x-1}$ such that $x_i = (i-1)\,\Delta x$, for $i = 1, 2, \ldots, N_x$. In addition, let

n^h denote an approximation to the solution n. We discretize the space (size) variable x and obtain the following continuous version of (5.6)

$$\begin{aligned}\frac{\partial n^h(x_i,t)}{\partial t} &= \frac{\theta(x_i)}{2}\int_0^{x_i} n^h(x_i-y,t)\,n^h(y,t)\,dy - \theta(x_i)\,n^h(x_i,t)\int_0^{\infty} n^h(y,t)\,dy,\\ n^h(x_i,0) &= \theta(x_i)\,c_0^h(x_i) = n_0^h(x_i),\end{aligned} \tag{5.8}$$

for $i = 1,2,\ldots,N_x$. To obtain a discrete version of the equation (5.8) we need to approximate the integrals in (5.8). For the discretization of these terms we use quadrature formulas:

$$\int_a^b f(y)\,dy \sim \sum_{j=1}^{N_q} f(x_j)w_j \tag{5.9}$$

where N_q is the number of quadrature points, the w_j are the appropriate weights and the x_j are the node points in the grid, if a closed Newton-Cotes formula is used (see e.g. [91]), or the quadrature nodes, otherwise. We allow different quadrature formulas and thus different weights for the collision integrals.

In order to approximate the convolution integral in (5.8), which for simplicity we denote by H_1, we use (5.9) which yields

$$H_1(x_i,t) := \theta(x_i)\int_0^{x_i} n^h(x_i-y,t)\,n^h(y,t)\,dy \sim \theta(x_i)\sum_{j=1}^{i} w_j\,n^h(x_i-x_j,t)\,n^h(x_j,t) \tag{5.10}$$

for $i = 1,2,\ldots,N_x$. For the numerical computation of H_1, we have used two different quadrature rules (both low order): trapezoidal and Simpson's rule. Note that a discrete coagulation equation that is obtained from (5.8) using (5.10) needs to be expressed only in terms of the size distribution at the node-points. In this sense, the choice of a uniform grid is rather convenient as in this case the size of a new aggregate, such as $x_i - x_j$ matches exactly one of the grid points, i.e. $x_i - x_j = (i-j)\,\Delta x = x_{i-j+1}$. However, when using a nonuniform grid (such as a geometric or logarithmic), the size $x_i - x_j$ usually falls between the grid points. For this reason, one needs to interpolate the distribution n^h between the nodes of the grid. An example of such an interpolation technique is provided below (for the discretization of H_2).

To approximate the second integral in (5.8), (which, for simplicity, we denote by H_2), we use two different quadrature rules: Simpson's and Gauss-Laguerre quadrature rules. The discretization of the integral H_2 by the Gauss-Laguerre quadrature rule reads as:

$$H_2(x_i,t) = \theta(x_i)\, n^h(x_i,t) \int_0^{\infty} e^{-y}[e^{y} n^h(y,t)]dy$$
$$\sim \theta(x_i) n^h(x_i,t)\Big(\sum_{k=1}^{m} \omega_k \exp(\zeta_k) n^h(\zeta_k,t) + \frac{(m!)^2}{(2\,m)!}\Big[e^{\xi} n^h(\xi,t)\Big]^{(2\,m)}(\xi)\Big),\ \xi > 0 \tag{5.11}$$

Here, m is the number of Gauss-Laguerre nodes, and ζ_k and ω_k are the Gauss-Laguerre nodes and weights, respectively. It is well known that the rule (5.11) is convergent if the function n^h satisfies the inequality $|n^h(x)| \leq x^{1+\rho}$, for some $\rho > 0$. Using Gauss-Laguerre rule requires some knowledge of the discretized solution n^h at the Gauss-Laguerre nodes ζ_k for $k = 1, ..., m$. Since the solution is known only at the node points x_i, $i = 1, 2, \ldots, N_x$ of the uniform grid, we need to resort to interpolation of the distribution function $n^h(\zeta_k, t)$ between the node points x_i of the grid. For this reason we use the following interpolation/extrapolation: If $\zeta_k \leq x_1 = 0$ then we choose $n^h(\zeta_k, t) = n^h(x_1, t)$. If $x_1 < \zeta_k < x_{N_x}$ then we use piecewise linear interpolation

$$n^h(\zeta_k,t) = \Big(1 - \frac{\zeta_k - x_{q-1}}{\Delta x}\Big) n^h(x_{q-1},t) + \frac{\zeta_k - x_{q-1}}{\Delta x} n^h(x_q,t),$$

where $\zeta_k \in (x_{q-1}, x_q]$, $q = 1, 2, \ldots N_x - 1$. This corresponds to the index q defined by

$$q = \operatorname{ceil}\Big(\frac{\zeta_k - x_{q-1}}{\Delta x}\Big) + 1,$$

where ceil(p) denotes the smallest integer greater than or equal to p. Finally, if $\zeta_k \geq x_{N_x}$ then we extrapolate $n^h(\zeta_k, t)$ according to the formula

$$n^h(\zeta_k,t) = \Big(1 - \frac{\zeta_k - x_{N_x}}{\Delta x}\Big) n^h(x_{N_x},t) + \frac{\zeta_k - x_{N_x}}{\Delta x} n^h(x_{N_x-1},t).$$

Remark 5.1 *A similar type of interpolation can be used to discretize the convolution-type integral H_1 in the case of a non-uniform grid, the modification being in ζ_k above being replaced by $x_i - x_j$. Hence, the distribution $n^h(x_i - x_j, t)$ is obtained from $n^h(x_s, t)$, where $s = 1, 2, \ldots, N_x$ by use of an interpolation as above.*

The numerical method described so far leads to a discrete version of the coagulation equation (5.6) and thus to a system of ODEs for the unknowns $n^h(x_i, t) =: n_i(t)$:

$$\frac{dn_i(t)}{dt} = \frac{\theta(x_i)}{2} \sum_{j=1}^{i} w_j\, n_{i-j+1}(t)\, n_j(t) - \theta(x_i)\, n_i(t) \sum_{j=1}^{N_x} \tau_j\, n_j(t) \tag{5.12}$$

for $i = 1, 2, \ldots, N_x$, where the initial condition $n_i(0) = n^h(x_i, 0) = \theta(x_i)\, c(x_i, 0)$ is given in the problem and the weights w_j and τ_j are implemented in Matlab.

It remains only to solve the resulting system of ODEs (5.12) to determine the unknown vector $[n_1(t), n_2(t), \ldots, n_{N_x}(t)]^T$. For the time-integration of the system of ODEs (5.12) we choose again a uniform grid t_k, $1 \leq k \leq N_t$ where $t_{N_t} = T_{max}$, with spacing $\Delta t = \frac{T_{max}}{N_t - 1}$ such that $t_k = (k-1)\,\Delta t$, for $k = 1, 2, \ldots, N_t$. We denote by $n_i^k = n^h(x_i, t_k)$ the value of the function n^h at the grid point $(x_i, t_k) \in [0, X_{max}] \times [0, T_{max}]$. For the time integration of the system (5.12) of ODEs, we use a variety of numerical schemes that include: explicit Forward-Euler method and Runge-Kutta method. For the latter, we make use of the **ode45** Matlab function. To verify the correctness of our numerical method, we compare the numerical solution with known explicit solutions in the absence of particle source terms. Although in Section 4.2 we obtained some asymptotic solutions for the coagulation equation (5.6) in the case of a bilinear kernel $K(x, y) = (\alpha + \beta\, x)\,(\alpha + \beta\, y)$ with α, $\beta > 0$, the initial conditions involve dirac delta functions which are not easy to implement numerically. For this reason, to test our numerical method we have only considered the case of a product kernel $K(x, y) = x\, y$, ($\alpha = 1$ and $\beta = 0$) without sources ($g(x, t) = 0$).

5.3.2 Experimental results

In this subsection we present some comparison results of the numerical and analytical size distributions. First, we consider the explicit solution given by Ernst et al [34]. Let the initial size distribution be $n(x, 0) = \exp(-x)$ and $g(x, t) = 0$. Then the exact solution of (5.6) is given by

$$n(x, t) = \frac{I_1(2\, x\sqrt{t})}{x\,\sqrt{t}}\; e^{-T\, x} \tag{5.13}$$

where $T = 1 + t$, for $t \leq 1$ and $T = 2\sqrt{t}$, for $t > 1$. Note that $T_{gel} = 1$. Also, I_1 is the modified Bessel function of the first kind [1]. To implement the modified Bessel function of the first kind numerically, we use the following approximations provided by Abramowitz and Stegun [1]:

$$I_1(x) \sim x \cdot \left(P_1 + P_2\, y^2 + P_3\, y^4 + P_4\, y^6 + P_5\, y^8 + P_6\, y^{10} + P_7\, y^{12}\right), \quad \text{if} \quad x \in [0, 3.75]$$

and

$$I_1(x) \sim \frac{e^x}{\sqrt{x}} \cdot \left(Q_1 + Q_2\, w + Q_3\, w^2 + Q_4\, w^3 + Q_5\, w^4 + Q_6\, w^5 + Q_7\, w^6 + Q_8\, w^7 + Q_9\, w^8\right),$$

if $x \in [3.75, \infty)$, where P_i, $i = 1, \ldots, 7$ and Q_j, $j = 1, \ldots, 9$ are given in ([1], p.378) and $y = x/3.75$, $w = 1/y$. For the discretization of the integral terms we use trapezoidal and Gauss-Laguerre rules respectively, whereas for the time-discretization we use fourth order Runge-Kutta method. This combination seems to yield accurate results when compared with other methods we tried.

First, we investigate the L^1 discrete error norm (numerical error):

$$E^h(t^k) = \sum_{i=1}^{N_x} |n_i^k - n(x_i, t^k)| \, \Delta x \tag{5.14}$$

where n denotes the exact solution to (5.6) and n_i^k the approximate solution. We have computed the discrete error (5.14) for a fixed $X_{max} = 100$ and using a successive number of points $N_x = 101, 201, 401$. The results are presented in Figure 5.7. As expected, the numerical error $E^h = \mathcal{O}((\Delta x)^2)$ is proportional to $(\Delta x)^2$ (before gelation occurs, so for $t < T_{gel} = 1$). Hence, the numerical scheme is second order accurate (in space).

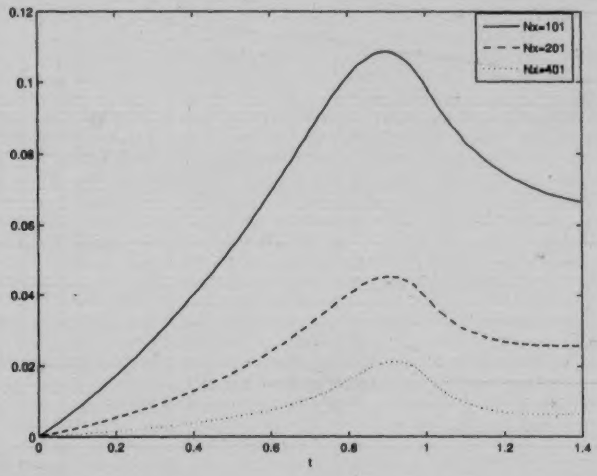

Figure 5.7: Time evolution of the numerical error in (5.14) for $X_{max} = 100$ using $N_x = 101, 201, 401$ points.

Next, we look at the time evolution of the numerical approximation n^h and analytical distributions n in (5.13) for the pure coagulation equation for a fixed size $x = 50$, where we choose a truncation parameter $X_{max} = 100$. The results are presented in Figure 5.8.

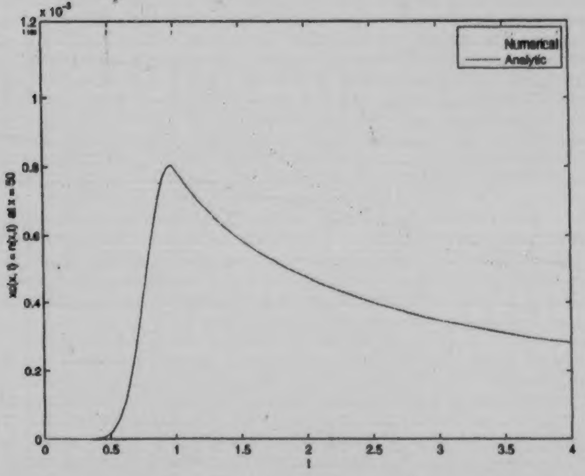

Figure 5.8: Time evolution of the particle size distribution $n(x,t)$ at $x = 50$, where $X_{max} = 100$.

As can be seen from Figure 5.8, there is good agreement between the numerical and exact solutions up to the gel-time $T_{gel} = 1$. However, after this time there is an almost constant deviation of the numerical solution from the exact solution: the numerical solution lies above the exact solution. This discrepancy between the solutions had been observed earlier in the work of Filbet et al [41] for the same rapidly growing coefficients $K(x,y) = x\,y$ using the finite volume method. To obtain accurate results, Filbet et al [41] suggest choosing a larger parameter X_{max}. The reason for this choice is that rapidly growing coefficients K induce a faster transfer of matter towards larger and larger sizes as the coalescence has the effect of shifting the distribution function $n(x,t)$ to the right as time goes by. On the other hand, these rapidly growing kernels also give rise to solutions that develop an algebraic tail upon the occurrence of gelation.

For comparison purposes we have also analyzed the time evolution of the discrete first and second moments $M_1^h(t)$, $M_2^h(t)$ and the exact corresponding moments of the solution $c(x,t)$. Figure 5.9 shows that the larger the truncation parameter the closer the discrete first moment $M_1^h(t)$ gets to the exact one $M_1(t)$.

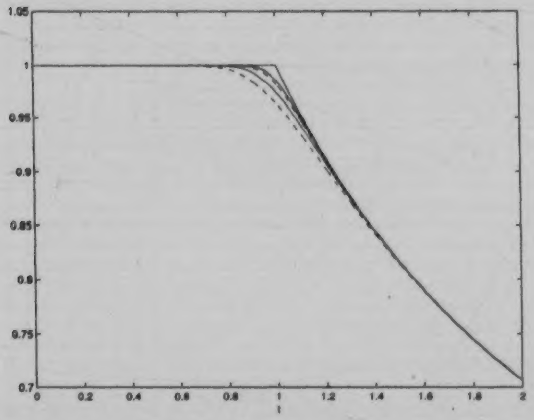

Figure 5.9: Time evolution of the discrete and exact moments $M_1^h(t)$ and $M_1(t)$ of the size distribution $c(x,t)$ for $X_{max} = 100, 200, 400, 600, \infty$ (left to right)

However, no matter how large we choose the parameter X_{max} the total mass decreases after the numerical gelation time. In addition, it seems difficult to capture the exact behaviour of the discrete $M_1^h(t)$ at $t = T_{gel}$ and estimate accurately the gelation time. As known from the articles of Ernst et al [34], Lushnikov [70] the gelation time corresponds to the first instance when the second moment of solution diverges. For this reason, one way to investigate the onset of gelation is to find an approximate interval of time t on which $1/M_2^h(t)$ is negligibly small. Our numerical observations of the discrete value $1/M_2^h(t)$ from repeated testing is that a very large truncation parameter X_{max} is needed to locate the gel-time. Similar conclusions have been pointed out in Filbet et al [41] who investigated the sudden growth of the second moment $M_2^h(t)$ and considered an X_{max} as large as 44110.

Our suggestion is that for the types of growing kernels considered in this section it is best to estimate the gelation time using Laplace transforms. To illustrate our idea, we return to the coagulation equation (5.6), formally apply Laplace transforms, and derive a first order PDE associated to (5.6). Based on the method of characteristics, solve the PDE for the Laplace transform and study the circumstances under which the system of characteristic equations can be inverted [15, 96]. This analysis leads to determining the gel-time, which in [15, 96] was proved to coincide with the so-called "breaking time", that is the first instance t at which the solution $D(\xi, t)$ of the following system of ODEs vanishes.

$$\frac{\partial^2 D}{\partial t^2}(\xi,t) - \frac{\alpha}{\beta}P(\xi,t)\frac{\partial D}{\partial t}(\xi,t) - \beta\frac{\partial G}{\partial z}(Z(\xi,t),t)D(\xi,t) = 0$$

$$\text{with initial conditions: } D(\xi,0) = 1; \ \frac{\partial D}{\partial t}(\xi,0) = \beta h'(\xi), \quad \text{where } \xi > 0$$

$$\frac{\partial P}{\partial t}(\xi,t) = \frac{\alpha}{2\beta}P^2(\xi,t) + \beta R(Z(\xi,t),t)$$

$$\text{with initial condition: } P(\xi,0) = \beta\big(h(\xi) - h(0)\big)$$

where $R(z,t) := G(Z(\xi,t),t) - G(0,t)$, and $Y(z,t)$ defines the Laplace transform of the distribution $n(x,t)$. In the system of ODEs above, $G(z,t)$ and $h(z)$ represent the Laplace transforms of the source $\theta(x)\,g(x,t)$, and $n(x,t)$, respectively. The system can be solved analytically in some special cases, while in general numerical methods need to be employed (we have used fourth order Runge Kutta methods). Table 5.1 presents the exact values where known and the range for computed gel-times for a few classes of sources and initial conditions.

$g(x,t)$	$c(x,0)$	Exact T_{gel}	Range for computed T_{gel}
0	$\exp(-x)/x$	1	$1 \pm 1e-4$
0	$\exp(-x)$	0.5	$0.5 \pm 1e-4$
0	$\delta(x-1)$	1	$1 \pm 1e-4$
$\exp(-x)$	$\exp(-x)/x$	?	$[0.67533, 0.67553]$
$\exp(-x)$	$\exp(-x)$	?	$[0.4351, 0.4352]$
$\exp(-x)$	$\delta(x-1)$	?	$[0.67533, 0.67553]$
$\delta(x)$	$\exp(-x)/x$	1	$1 \pm 1e-4$
$\delta(x)$	$\exp(-x)$	0.5	$0.5 \pm 1e-4$
$t\exp(-x)$	$\exp(-x)/x$	?	$[0.45825, 0.45835]$
$t\exp(-x)$	$\exp(-x)$	?	$[0.09991, 0.09993]$

Table 5.1: Numerical and analytical experiments on the gelation time using Laplace transform methods.

5.3.3 Comparison with finite volume methods

To verify our numerical method we compare the numerical solution proposed in Section 5.3.1 with the corresponding solution obtained by Filbet et al [41] using the finite volume method for the same choice of parameters as in 5.3.2 (or the same exact solution (5.13)). The results of the comparison of the numerical methods are presented in Figure 5.10. We obtain the same numerical results with the collocation method in Section 5.2.

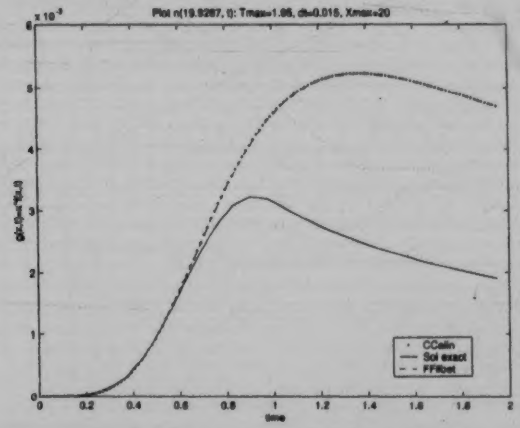

Figure 5.10: Time evolution of the numerical and exact distribution $n(x,t)$ at $x =$ 19.9287

5.3.4 Proposed improvements in the numerical scheme

In this subsection we propose two ways of improving the accuracy of the numerical scheme and thus lowering the numerical error that we get when truncating the problem to a finite domain and approximating the improper integral. The methods that we propose below are based on estimates of the improper integral in (5.6).

(a) Use of zeroth and first moments of the solution

In the attempt to lower the error that we obtain in the numerical solution, we have closely analysed the improper integral in the coagulation equation (5.6). Based on the form of the coagulation kernel K at the beginning of Section 5.3, the improper integral is a linear combination of the zeroth and first moments, so the coagulation equation (5.6) can be expressed in the following form

$$\frac{\partial n}{\partial t}(x,t) = \frac{\theta(x)}{2}\int_0^x n(x-y,t)n(y,t)\,dy - \theta(x)\,n(x,t)N(t) + \theta(x)\,g(x,t) \qquad (5.15)$$

where $N(t) = \alpha\, M_0(t) + \beta\, M_1(t)$. The truncation of the infinite domain to a finite upper limit clearly leads to an underestimation of $N(t)$ which reduces (5.6) to an approximation of this equation over a finite domain. Due to the finite computational domain $[0, X_{max}]$ that we use in the numerical solution and the nature of the equation (5.6), it is clear that particles within the finite domain interact with particles outside the computational domain. Moreover, due to the rapidly growing coefficients K considered in this section, more particles are formed outside the computational domain. Hence, unavoidable errors are introduced into the computed distribution and in particular into the improper integral(s) in equation (5.15).

To demonstrate that the effect of truncation on the improper integral is one of the sources of error in the numerical scheme, we investigate the possibility of lowering the error in the improper integral(s). For this purpose, we look at ways of coupling the equation (5.15) with corresponding ODEs (or general algebraic formulas) for the function $N(t)$. First, we consider a few special classes of initial conditions $c_0(x)$ for which explicit general formulas for $N(t)$ are available. The results of our experiments show that if instead of numerically approximating the zeroth and first moments as in 5.3.1, one couples (5.15) with an explicit formula or a correspondent ODE satisfied by $N(t)$, then one obtains excellent agreement between the numerical and explicit solution for a very large interval of time and large particle sizes.

To illustrate the idea presented above we consider the coagulation kernel $K(x, y) = x\,y$, and no sources ($g(x,t) = 0$). In this case, the explicit solution is given by (5.13). The time evolution of the particle size distribution $n(x,t)$ at $x = X_{max}$ is illustrated in Figure 5.11. In this instance, the function $N(t) = M_1(t)$ is known explicitly as: $M_1(t) = 1$, if $t \leq 1$ and $M_1(t) = 1/\sqrt{t}$, if $t > 1$. For the discretization of the convolution integral in (5.15) we have used Simpson's rule.

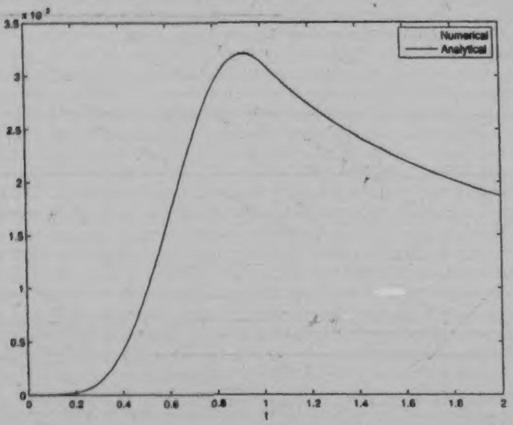

Figure 5.11: Time evolution of the approximated and exact distribution $n(x,t)$ using (a) for $x = X_{max} = 20$.

Figure 5.11 shows that the numerical solution is in excellent agreement with the exact solution for the truncation parameter $x = X_{max} = 20$. Therefore, such a coupled system yields accurate results and is not expensive computationally (no unnecessarily large truncation parameters are needed for the numerical solution to converge to the exact one). We have also looked at larger truncation parameters and obtained accurate numerical results. This improvement in the numerical solution is anticipated at the beginning of (a). A few possible explanations for such an improvement are provided below. On the one hand, the truncation of the infinite domain to a finite upper limit X_{max} results in an underestimation of the i^{th} moment of the solution in (5.15) by an amount

$$M_i^{tde}(t) = \int_{X_{max}}^{\infty} x^i \, c(x,t) \, dx$$

where $M_i^{tde}(t)$ represents the error that occurs in the i^{th} moment due to the truncation of the domain. On the other hand, we have already proved in some cases (see Sections 4.2, 4.3), that the distribution function $c(x,t)$ converges (asymptotically) to zero at sufficiently large particle sizes x. Thus, one has to choose a sufficiently large value for X_{max} so that this error is negligibly small. However, one has to carefully select the values of X_{max} so that they are not unnecessarily large as the distribution functions have tail regions that are difficult to represent. In addition, due to the very small values that these functions can take at large sizes they are computationally expensive to converge.

Gelbard and Seinfeld [48] were the first to provide a method of selecting appropriate upper limits X_{max} of the domain. Their approach is based on the concept of "finite domain error". Let

$$FDE_i(t) = \frac{\int_0^\infty x^i\, c(x,t)\, dx}{M_i^{tde}(t)}.$$

The authors select X_{max} such that $FDE_0(t)$ and $FDE_1(t)$ do not differ appreciably from unity. As authors acknowledge, this approach is restricted to cases where an analytical expression for $M_i^{tde}(t)$ is available. However, to investigate the onset of gelation, the second moment M_2 is preferred. A systematic method for choosing the values of X_{max} is suggested in Nicmanis et al [77] for the steady-state population balance equations. The authors suggest that selection of X_{max} be made to ensure that $M_2 > 0.999$. This yields the additional criteria $M_0 > 0.999$, $M_1 > 0.999$. However, in the criterion suggested in [77] the quantities M_i, $i = 0, 1, 2$ are constants, as $c(x,t) = c(x)$.

Another explicit solution for which we have shown the improvement **(a)** on the accuracy is the solution in Example 4.16. For this purpose, we choose in Example 4.16 the following parameters: $\alpha = 1$, $\beta = 0$, $K(x,y) = x\,y$, the initial condition $n_0(x) = k\, e^{-\sigma x}\, I_1(m\,x)/x$ and the source function

$$g(x,t) = H_0\, \frac{k\, e^{-x(Q(t)+\sigma)}\, I_1(m\,\sqrt{S(t)}\,x)}{x^2}\, S(t)^{2a-5/2}, \tag{5.16}$$

where $S(t) = \left(1 + \frac{k}{m}\, t\right)^2$. Then the exact solution to (5.2) is given as in Example 4.16:

$$n(x,t) = \frac{k\, e^{-(Q(t)+\sigma)\,x}\, I_1(m\,\sqrt{S(t)}\,x)}{x} \tag{5.17}$$

where the total mass $M_1(t) = Q'(t)$ is defined in Example 4.16. Our numerical and analytical results are represented for $k = m = \sqrt{\sigma^2 - \sigma_0^2} = \sqrt{3}$, $\sigma = 2$, $\sigma_0 = 1$, $X_{max} = 50$ and two different cases of sources $g(x,t)$. In Figure 5.12 we represent the time evolution of the numerical and exact solutions in the case $g \equiv 0$ (no sources), which corresponds to $H_0 = 0$, and $a = 1/2$. In this case the gelation time is given by the formula $T_{gel} = \sigma_0\, m/((\sigma - \sigma_0)\, k) = 1$. In Figure 5.13, we sketch the solutions in the presence of source terms, we choose $H_0 = k/m = 1$, so $a = 1$. Here, the gelation time is given by the formula $T_{gel} = (m/k)\,\left(\sqrt{(\sigma + \sigma_0)/(\sigma - \sigma_0)} - 1\right) = \sqrt{3} - 1$.

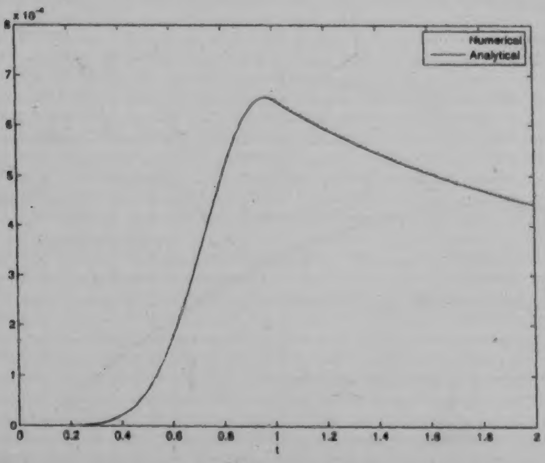

Figure 5.12: Time evolution of the numerical and exact distribution (5.17) using **(a)** for $x = X_{max} = 50$ and $g(x,t) = 0$.

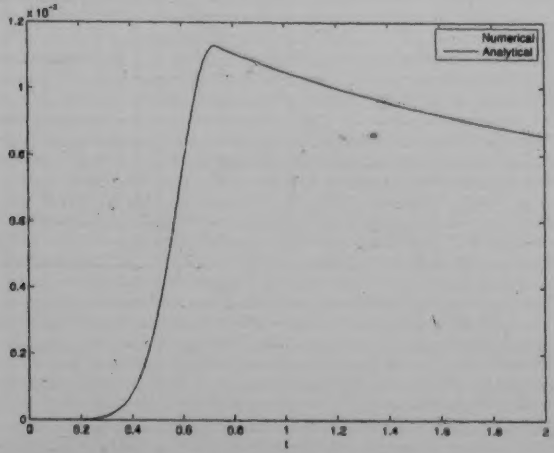

Figure 5.13: Time evolution of the numerical and exact distribution (5.17) using **(a)** for $x = X_{max} = 50$ and $g(x,t) > 0$ as in (5.16).

Our method in **(a)** can be applied to the pure coagulation equation ($g \equiv 0$) and a larger class of collision kernels $K(x,y) = (\alpha + \beta\, x)\,(\alpha + \beta\, y)$, ($\alpha \geq 0$, $\beta > 0$). One needs only to couple (5.15) with the general formula for $N(t)$ obtained by Shirvani and van Roessel [89]. The authors derived a general formula for the total mass $M_1(t)$:

$$M_1(t) = M_1(0) + \frac{1}{\beta} \int_0^{\xi_0(t)} h'(\rho)\, e^{-\frac{\alpha}{\beta}\rho}\, d\rho, \quad \text{for all time } t \geq 0,$$

where $\xi_0(0) = 0$, for $0 \leq t < T_{gel}$ and

$$\xi_0'(t) = \frac{\beta^2\, h'^2(\xi_0)(t)}{\beta\, h''(\xi_0(t)) - \alpha\, h'(\xi_0(t))/2}\, e^{-\frac{\alpha}{\beta}\xi_0(t)}, \quad \text{for} \quad t \geq T_{gel}$$

subject to the initial condition $\xi_0(T_{gel}) = 0$, where $T_{gel} = -1/(\beta\, h'(0))$ and $h(z)$ represents the Laplace transform of the initial distribution $n(x, 0)$. An explicit formula for $N(t)$ that is valid up to the gel-time T_{gel} is given by $N'(t) = -\alpha\, N^2(t)/2$. To obtain a general formula for $N(t)$ for all time $t \geq 0$, one can use the approach in Example 4.10. Use $M_0'(t) = -\frac{\alpha}{2} N^2(t)$, for all $t \geq 0$.

The numerical computations suggested in **(a)** are performed in combination with analytical solutions for $N(t)$. Future work extends the proposed improvement **(a)** to the general case $\alpha \geq 0$ and $\beta > 0$, where $N(t)$ cannot be solved analytically. In these cases we intend to solve the coupled system of equations (5.15) to obtain the numerical solution to $\tilde{n}^k$ (5.15) by successive approximations as follows

1. Choose a uniform partition x_i of the computational domain $\Omega = [0, X_{max}]$.
2. Calculate $\tilde{n}^0(x_i, t) = \tilde{n}_i^0(t) = n(x_i, 0)$ (intial condition) at the grid nodes.
3. For $k = 1, \ldots, N_{max}$

Approximate $\tilde{N}^k(t) = \int_0^{\infty} \tilde{n}^{k-1}(y, t)\, dy$ by quadrature rules

$$\frac{\partial \tilde{n}^k}{\partial t}(x, t) + \theta(x)\, \tilde{n}^k(x, t) \tilde{N}^k(t) = \frac{\theta(x)}{2} \int_0^x \tilde{n}^{k-1}(x - y, t) \tilde{n}^{k-1}(y, t)\, dy + \theta(x)\, g(x, t)$$

4. if $\max |\tilde{n}^k(x, t) - \tilde{n}^{k-1}(x, t)| > Tol$

update the time step $t = t + \Delta t$ until you have reached T_{max} (5.18)

where for simplicity we denote the approximation n^h of the solution n to (5.15) as $n^h := \tilde{n}$ and $\tilde{N}$ represents a numerical approximation of $N(t)$. In the scheme presented above, N_{max} is the maximum number of iterations, and Tol is some prescribed tolerance.

The technique suggested above has been successfully used in the literature to numerically solve certain Volterra integral equations. In fact, Melzak [74] proved theoretical results for coagulation equations using the Picard method of successive approximations, which can be used for initial stages of the evolving spectrum. However, a similar technique as in Section 5.2 can be used to provide good numerical results (or qualitative behaviour of solutions for large sizes). If one is interested in defining the entire history of an evolving spectrum then numerical solutions have to be combined with asymptotic solutions as suggested by Drake [25]. Our second suggestion in **(b)** is based on the use of combined numerical methods and asymptotic solutions and thus it is more general.

(b) Use of the asymptotic solution $c(x,t)$ at large sizes x

The method that we propose in this subsection is also intended to improve the accuracy of the numerical results in 5.3.1. This method is based on taking advantage of the asymptotic behaviour of solutions in Chapter 4 at large sizes into the numerical scheme. This second method is provided as a means of lowering the numerical error that we obtained in 5.3.1 due to the underestimation of the second integral. More precisely, this method takes into account the asymptotic behaviour of the solution $c(x,t)$ for large x which in turn allows us to split the improper integral in (5.13) into two integrals:

$$\int_0^\infty n(x,t)\,dx = \int_0^{X_{max}} n(x,t)\,dx + \int_{X_{max}}^\infty n(x,t)\,dx.$$

For the discretization of the first integral we use quadrature rules (as in 5.3.1). However, for the second integral we make use of the asymptotic behaviour of the solution for large x and either calculate it analytically (if possible) or approximate it.

The selection of the truncation parameter X_{max} plays an important role as it affects the computational time. Between the two methods presented in part **(a)** for selecting the upper bound X_{max} we have chosen the one based on M_1^{tde}. Alternatively, one can also make use of the method suggested by Drake [25], and determine the lower bound x_m on the particle sizes x for which the ratio between the exact solution of (5.15) written in the form of an infinite series (using the approach suggested by Scott [94]) and the asymptotic solution (obtained by the saddle point method) remains within 1% of unity. Drake [25] showed that if the coagulation kernel is $K(x,y) = x\,y$, and for a family of initial gamma distributions of the form

$$c_0(x) = \frac{(\nu+1)^{\nu+1}}{\Gamma(\nu+1)}\,x^\nu\,e^{-x(\nu+1)}$$

If $x > x_m$ then the asymptotic solutions represent the exact solution to within less than 1% error. Here x_m is defined by

$$x_m = \frac{z_m \left(2T\right)^{-\left(\frac{1}{\nu}+3\right)}}{\nu + 3} \left(\frac{\nu + 2}{\nu + 1}\right)^{\frac{\nu+2}{\nu+3}}$$

where $T = 1 - M_0(t)$. For example, if $\nu = 1$ then it was found that $z_m = 7$ and as ν increases, x_m increases. Future work will investigate more general ways of choosing X_{max} that are based on moving mesh techniques. In this case the upper limit X_{max} moves with time and does not rely on analytical results.

For illustrating the results using the method **(b)**, we consider the asymptotic solution (4.58) obtained in Example 4.3 for λ large (in our case we denote $x = \lambda$) and $t \geq 0$. Figure 5.14 shows an excellent agreement between the numerical and analytical solution for a truncation parameter as small as $X_{max} = 50$ and a relative large interval of time $t \in [0, 5]$. In the attempt to validate our combined numerical and asymptotic method in **(b)** we have also considered the linear kernels and obtained that the numerical solution is in perfect agreement with the exact solution.

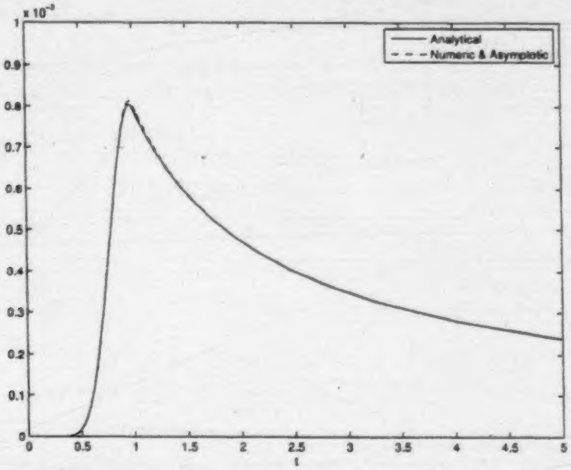

Figure 5.14: Time evolution of the approximated and exact distributions (5.13) using **(b)** at $x = X_{max} = 50$, for $g(x, t) = 0$.

Conclusions

In this chapter we have suggested a few numerical methods for solving the coagulation equations in the absence/presence of particle source terms. We have divided our presentation of the methods in three sections. In Section 5.1 we have reviewed some of the deterministic methods that have been developed so far in the literature of coagulation. On the basis of the conclusions of these studies, the discretized population balance equations method of Litster et al [67], the pivot method of Kumar and Ramkrishna [59, 60], and the Galerkin and orthogonal collocation on finite element methods were found to be the most accurate and stable numerical techniques. Despite their predicted accuracy there are some common problems associated to the numerical solution of these equations. These include: the inaccurate calculation of the particle size distributions for highly aggregating processes, numerical instabilities, domain errors for high-order coagulation kernels (specially those related to gelation phenomenon). Due to the numerical difficulties of these methods and their limitations, improved methods are of interest.

Our main purpose, in Section 5.2 is to provide some improved methods that deal with general, though bounded coagulation kernels. For these types of kernels, we focus on two numerical methods: weighted residual methods (collocation) and adapted power series methods. The adapted power series turns out to be quite a reliable method for obtaining qualitative information about the numerical solution when compared to the exact known solution and the collocation method (even when we use only terms up to t^2 in the series). One main advantage of using adapted power series over collocation methods is related to the computational time. Even though the collocation method requires integration only at the nodal points and seems to have good accuracy even with linear elements, it is computationally expensive.

In Section 5.3 we provide some numerical results for kernels that increase sufficiently fast, taking into account the presence of particle source terms. The method that we provide in this section is based on a direct discretization of the coagulation equation; followed by quadrature methods for the integral terms (based on Trapezoidal, Simpson's and Gauss-Laguerre quadrature) and time-integration of the system of ODEs. The method becomes more accurate when we combine the numerical scheme with the knowledge of the total mass (directly or through ODEs) or the asymptotic behaviour of solutions at large sizes. As pointed out in Chapter 4, for the coagulation kernels $K(x,y) = (\alpha + \beta x)(\alpha + \beta y)$, one can derive a new family of similarity (group invariant) solutions for the coagulation equations. These solutions depend on the function $Q(t)$ and thus on $N(t)$, which in turn satisfies an ODE. For some special cases, one can solve the ODE and deduce $N(t)$ or some general formulas and thus derive explicit or asymptotic solutions $n(x,t)$ for (5.6) at large sizes and all time $t \geq 0$.

In general, one needs to solve the ODE for $N(t)$ (or $Q(t)$ in the notation of Chapter 4) using numerical methods. Therefore, the methods in the subsections **(a)** and **(b)** prove to be quite useful in deriving a class of accurate numerical solutions to (5.6).

Chapter 6

Summary and Future directions

6.1 New and old solutions to the coagulation equation

In this section we provide a brief summary of the similarity solutions we derived in Sections 4.2, 4.3. Our summary is divided into a few subsections that include explicit, asymptotic and power series solutions for a few types of coagulation kernels $K(\lambda, \mu, t) = 1, \alpha^2(t),\ \lambda\,\mu,\ \beta^2(t)\,\lambda\,\mu,\ (\alpha + \beta\,\lambda)\,(\alpha + \beta\,\mu)$. We summarize the solutions we obtained in Chapter 4 in the form of tables. Almost all the solutions are new/general family of solutions in the literature of coagulation or they are more general family of solutions. All these solutions have been derived by using our *direct* and *indirect* methods in Chapter 4. For more details and derivation of the examples we present in the tables below see Section 4.2, 4.3.

6.1.1 $K(\lambda,\mu,t) = 1$ and $g(\lambda,t) \geq 0$

Parameters	NEW solution (Example 4.15)	Smoluchowski's solution
$c_0(\lambda)$	$e^{-\lambda}$	$e^{-\lambda}$
$R(t)$	non-decreasing, $R(t) \geq 0$, and $R(0) = 0$	0
$T(t)$	$\frac{2}{2+\int_0^t e^{R(\tau)}\,d\tau}$	$\frac{2}{2+t}$
$g(\lambda,t)$	$R'(t)\,T^2(t)\,e^{R(t)-\lambda T(t)}$	0
$c(\lambda,t)$	$T^2(t)\,e^{R(t)-\lambda T(t)}$	$\frac{4}{(2+t)^2}\,e^{-\frac{2\lambda}{2+t}}$
$M_1(t)$	$e^{R(t)}$	1
T_{gel}	∞ (no gelation)	∞ (no gelation)

Table 6.1: Explicit solutions for the kernel $K(\lambda,\mu,t) = 1$

6.1.2 $K(\lambda,\mu,t) = \alpha^2(t)$ and $g(\lambda,t) \geq 0$

Parameters	NEW solution (Example 4.12 (i))
Conditions	$r,\ m,\ q > 0,\ r \neq 1,\ a\,(r-1) > 0$
$K(\lambda,\mu,t)$	$\frac{q}{m}\,(1+r\,t)^{\frac{(b-a-1)\,(r-1)}{r}}$, $a\,b$ are arbitrary constants.
$c_0(\lambda)$	$m\,e^{-q\,\lambda}$
$g(\lambda,t)$	$a\,m\,(r-1)\,(1+r\,t)^{\frac{(a+4b-1)\,(r-1)}{r}}\,e^{-q\,(1+r\,t)^{\frac{b\,(r-1)}{r}}\,\lambda}$
$c(\lambda,t)$	$m\,(1+r\,t)^{\frac{(a+2b)\,(r-1)}{r}}\,e^{-q\,(1+r\,t)^{\frac{b\,(r-1)}{r}}\,\lambda}$
$M_1(t)$	$\frac{m}{q^2}\,(1+r\,t)^{\frac{a\,(r-1)}{r}}$
T_{gel}	∞ (no gelation)
Remarks	If $a = 0,\ b = 1 \Rightarrow \begin{cases} r = \frac{1}{2},\ q = m,\ g \equiv 0,\ K \equiv 1 \\ \text{Solution: } c(\lambda,t) = \frac{4m}{(2+t)^2}\,e^{-\frac{2m}{2+t}\,\lambda} \end{cases}$

Table 6.2: Explicit solutions for the time-dependent kernel $K(\lambda,\mu,t) = \alpha^2(t)$

Parameters	NEW solution (Example 4.12 (ii))
Conditions	$m,\ q > 0,\ a \leq 0$
$K(\lambda, \mu, t)$	$\frac{q}{m}\, e^{(a+\frac{1}{2})t}$, a an arbitrary constant.
$c_0(\lambda)$	$m\, e^{-q\lambda}$
$g(\lambda, t)$	$-a\, m\, e^{-(a+1)\,t}\, e^{-q\,\lambda\, e^{-t/2}}$
$c(\lambda, t)$	$m\, e^{-(a+1)\,t}\, e^{-q\,\lambda\, e^{-t/2}}$
$M_1(t)$	$\frac{m}{q^2}\, e^{-a\,t}$
T_{gel}	∞ (no gelation)

Table 6.3: Explicit solutions for the time-dependent kernel $K(\lambda, \mu, t) = \alpha^2(t)$

6.1.3 $K(\lambda, \mu, t) = \lambda\, \mu$ and $g(\lambda, t) \geq 0$

Parameters	NEW solution (Example 4.1)
Conditions	$A,\ p,\ q,\ a > 0$
Definitions	$\alpha_0 := \left(\frac{A}{p}\right)^{\frac{p}{p+1}}$
$\lambda\, c_0(\lambda)$	$\begin{cases} \text{given by the inverse Laplace transform of } \quad h(x) \\ h(x) \text{ satisfies the algebraic eq.} \quad A\,[h(x)]^{-1/p} + q\,h(x) - (x+a) = 0 \end{cases}$
$g(\lambda, t)$	0
$c(\lambda, t)$	$\frac{1}{\sqrt{2\pi}}\, \sqrt{\frac{\alpha_0\, p}{p+1}}\, t^{-\frac{(2p+1)}{2\,(p+1)}}\, \lambda^{-5/2}\, e^{-\left(Q(t)+a-\alpha_0\,(p+1)\,t^{1/(p+1)}\right)\,\lambda}$
$Q(t)$	$\begin{cases} h(0)\,t, \text{ for } t \in [0, T_{gel}) \\ -a + \alpha_0\,(p+1)\,(t+q)^{-\frac{p}{p+1}}, \text{ for } t \geq T_{gel} \end{cases}$
$M_1(t)$	$\begin{cases} h(0), \text{ for } t \in [0, T_{gel}) \\ \alpha_0\,(t+q)^{-\frac{p}{p+1}}, \text{ for } t \geq T_{gel} \end{cases}$
T_{gel}	$\frac{A}{p}\,[h(0)]^{-\frac{p+1}{p}} - q$
Notes	We recover asymptotic Eq. [3.13] in Ernst et al. [34]; Our asymptotic solution is more general than Eq. [3.13]

Table 6.4: Asymptotic large size ($\lambda \to \infty$) solutions for $K(\lambda, \mu, t) = \lambda\, \mu$

Parameters	NEW solution (Example 4.3)	NEW solution (Example 4.4)
Conditions	$A,\ p,\ q,\ a > 0$	$\gamma_0,\ \rho > 0$
Definitions	$\alpha_0 := \left(\frac{A}{p}\right)^{\frac{p}{p+1}},\ \beta_0 := \left(\frac{A}{a}\right)^{p}$	
$c_0(\lambda)$	$\frac{A^p\,\lambda^{p-2}\,e^{-a\,\lambda}}{\Gamma(p)}$	$\frac{\gamma_0}{\lambda}\,\delta(\lambda-\rho)$
$g(\lambda,t)$	0	0
$c(\lambda,t)$	$\sqrt{\frac{\alpha_0\,p}{2\,\pi\,(p+1)}}\ t^{-\frac{(2p+1)}{2\,(p+1)}}\,\lambda^{-5/2}e^{-(Q(t)+a-\alpha_0(p+1)t^{1/(p+1)})\,\lambda}$	$\frac{\lambda^{-5/2}}{t\sqrt{2\pi\,\rho}}\,e^{-\left(Q(t)-\frac{1+\ln(\gamma_0\,\rho\,t)}{\rho}\right)\lambda}$
$Q(t)$	$\begin{cases}\beta_0\,t, \text{ for } t\in[0,T_{gel}) \\ -a+\alpha_0\,(p+1)\,t^{-\frac{p}{p+1}}, \text{ for } t\geq T_{gel}\end{cases}$	$\begin{cases}\gamma_0\,t, \text{ for } t\in[0,T_{gel}) \\ \frac{1+\ln(\gamma_0\,\rho\,t)}{\rho}, \text{ for } t\geq T_{gel}\end{cases}$
$M_1(t)$	$\begin{cases}\beta_0, & \text{for } t\in[0,T_{gel}) \\ \alpha_0\,t^{-\frac{p}{p+1}}, \text{ for } t\geq T_{gel}\end{cases}$	$\begin{cases}\gamma_0, \text{ for } t\in[0,T_{gel}) \\ \frac{1}{\rho\,t}, \text{ for } t\geq T_{gel}\end{cases}$
T_{gel}	$\frac{A}{p}\,(\beta_0)^{-\frac{p+1}{p}}$	$\frac{1}{\gamma_0\,\rho}$
Remarks	$\begin{cases}A=a=p>0 \Rightarrow \text{ Eq. [3.13] in [34]} \\ A=p=a=1 \Rightarrow \text{ Sol. [3.5a] in [34]}\end{cases}$	We recover [3.8a] in [34]
Notes	We recover [3.13] in Ernst et al. [34]	Our sols. are more general

Table 6.5: Asymptotic large size ($\lambda \to \infty$) solutions for $K(\lambda,\mu,t)=\lambda\,\mu$

Parameters	NEW solution (Example 4.16 **(i)**)	NEW solution (Example 4.14 **(ii)**)
Conditions	$\sigma,\ k,\ m,\ p,\ H_0\geq 0,\ a\geq\frac{1}{2}$	$k,\ p>0,\ H_0=0,\ a=\frac{1}{2},\ \sigma\geq m>0$
Definitions		$\sigma_0=\sqrt{\sigma^2-m^2}$
$S(t)$	$\left[1+\frac{k}{m}\,(3-2\,a)\,t\right]^{\frac{2}{3-2a}}$	$1+\frac{2\,k}{m}\,t$
$c_0(\lambda)$	$\frac{k\,e^{-\lambda\,\sigma}\,I_1(m\,\lambda)}{\lambda^2}$	$\frac{k\,e^{-\lambda\,\sigma}\,I_1(m\,\lambda)}{\lambda^2}$
$g(\lambda,t)$	$H_0\,\frac{k\,e^{-\lambda\,(Q(t)+\sigma)}\,I_1(m\,\lambda\,\sqrt{S(t)})}{\lambda^2}\,S(t)^{2a-5/2}$	0
$Q(t)$	given by the I.V.P. (4.294)	$\begin{cases}\frac{k}{m}\,(\sigma-\sigma_0)\,t, \text{ for } t\in[0,T_{gel}) \\ m\,\sqrt{1+\frac{2kt}{m}}-\sigma, \text{ for } t\geq T_{gel}\end{cases}$
$c(\lambda,t)$	$\frac{k\,e^{-\lambda\,(Q(t)+\sigma)}\,I_1(m\,\lambda\,\sqrt{S(t)})}{\lambda^2\,[S(t)]^{1-a}}$	$\frac{k\,e^{-\lambda\,(Q(t)+\sigma)}\,I_1\left(m\,\lambda\,\sqrt{1+\frac{2\,k}{m}\,t}\right)}{\lambda^2\,\sqrt{1+\frac{2\,k}{m}\,t}}$
$M_1(t)$	given by an IVP obt. from (4.294)	$\begin{cases}\frac{k\,(\sigma-\sigma_0)}{m}, \text{ for } t\in[0,T_{gel}) \\ \frac{k}{\sqrt{1+\frac{2k}{m}\,t}}, \text{ for } t\geq T_{gel}\end{cases}$
T_{gel}	use numerical methods (future work)	$\frac{\sigma_0\,m}{k(\sigma-\sigma_0)}$

Table 6.6: Explicit solutions for $K(\lambda,\mu,t)=\lambda\,\mu$

6.1.4 $K(\lambda, \mu) = \lambda\, \mu$ and $g(\lambda, t) > 0$

Parameters	NEW solution (Example 4.16 (ii))
Conditions	$k,\, m,\, \sigma > 0,\ \sigma \geq m > 0$
Definitions	$\sigma_0 = \sqrt{\sigma^2 - m^2}$
$c_0(\lambda)$	$k\, e^{-\lambda \sigma}\, \frac{I_1(m\, \lambda)}{\lambda^2}$
$g(\lambda, t)$	$\frac{k^2\, e^{-\lambda\, (Q(t)+\sigma)}\, I_1((k\, t+m)\, \lambda)}{\lambda^2\, (k\, t+m)}$
$Q(t)$	$\begin{cases} \frac{k}{m^2}\, (\sigma - \sigma_0) \left(\frac{k}{2}\, t^2 + m\, t\right), & \text{for} \quad t \in [0, T_{gel}) \\ k\, t + m - \sigma, & \text{for} \quad t \geq T_{gel} \end{cases}$
$c(\lambda, t)$	$\frac{k\, e^{-\lambda\, (Q(t)+\sigma)}}{\lambda^2}\, I_1\big((k\, t + m)\, \lambda\big)$
$M_1(t)$	$\begin{cases} \frac{k}{m^2}\, (\sigma - \sigma_0)\, (kt + m), & \text{for} \quad t \in [0, T_{gel}) \\ k, & \text{for} \quad t \geq T_{gel} \end{cases}$
T_{gel}	$\frac{m}{k} \left(\sqrt{\frac{\sigma+\sigma_0}{\sigma-\sigma_0}} - 1\right)$

Table 6.7: Explicit solution for $K(\lambda, \mu, t) = \lambda\, \mu$

Parameters	NEW solution (Example 4.7)
Conditions	$\begin{cases} p,\, q > 0,\, m < -1,\, \left\lvert \ln\left(-\frac{2}{A^2\,(1+m)}\right)\right\rvert > (1-m)\, \sqrt{q}, \text{ where} \\ A = \frac{\exp\left(\frac{(1-m)}{2}\, \sqrt{q}\right)}{p\left(\frac{a}{\sqrt{q}}\right)^{\frac{1-m}{2}} + \sqrt{p^2 \left(\frac{a}{\sqrt{q}}\right)^{1-m} + \frac{2}{1+m}}} \end{cases}$
$\lambda\, c_0(\lambda)$	$\begin{cases} \text{given by the inverse Laplace transform of} \quad h(x) \quad \text{defined as} \\ h(x) = \frac{p}{q} \left(x + a - \sqrt{(x+a)^2 + \frac{2\, q^{-\frac{(m-1)}{2}}}{p^2\,(1+m)}\, (x+a)^{1+m}}\right) \end{cases}$
$g(\lambda, t)$	$\frac{\lambda^{-m-2}\,(2\, p\, t+q)^{-\frac{3+m}{2}}}{\Gamma(-m)}\, e^{-\lambda\, (Q(t)+a)}$
$Q(t)$	$\begin{cases} \sqrt{2pt+q} \left(\frac{A^2\, \exp\left(-(1-m)\sqrt{2pt+q}\right) - \frac{2}{1+m}}{2\, A\, p\, \exp\left(-\frac{(1-m)}{2}\, \sqrt{2pt+q}\right)}\right)^{2/(1-m)} - a, & \text{for} \quad t \in [0, T_{gel}) \\ \sqrt{2pt+q} \left(-\frac{2}{p^2\,(1+m)}\right)^{1/(1-m)} - a, & \text{for} \quad t \geq T_{gel} \end{cases}$
$c(\lambda, t)$	$\frac{p\, e^{-(Q(t)+a)\, \lambda}}{\lambda^2\, (2pt+q)} \sum_{k=1}^{\infty} \frac{(2k-2)!}{2^{2k-1}\, k!(k-1)!} \left(\frac{2\,(2pt+q)^{\frac{1-m}{2}}}{p^2\,(-1-m)}\right)^k \frac{1}{\Gamma((1-m)k-1)}\, \lambda^{(1-m)\, k}$
T_{gel}	$\frac{1}{2\, p(1-m)^2} \left[\ln\left(-\frac{2}{A^2\,(1+m)}\right)\right]^2 - \frac{q}{2p}$

Table 6.8: Formal series solution for $K(\lambda, \mu, t) = \lambda\, \mu$

Parameters	NEW solution (Example 4.8)
Conditions	$\frac{c_3}{c_2} > \sqrt{2}$
Definitions	$\begin{cases} w(s) > 0, \ \forall\, s \\ w'(s) \text{ completely monotonic in } s, \forall\, s \\ \lim_{s\to\infty} w'(s)\, e^{-w(s)} = 0 \text{ and } \lim_{s\to\infty} w(s) = \infty \end{cases}$
Examples	$\begin{cases} \textbf{(a) } w(s) = s^{\alpha}, & \text{where } \alpha \in (0,1] \\ \textbf{(b) } w(s) = \ln(1+(s+a)^{\beta}), & \text{where } \beta \in (0,1],\ a > 0 \text{ arbitrary} \end{cases}$
$h(x)$	$\frac{c_3}{c_2}\left(1 - \sqrt{1 - \frac{2c_2^2}{c_3^2}\, e^{-w(x)}}\right)$
$G(x,t)$	$w'(x - \frac{c_3}{c_2}\, t)\, e^{-w(x - \frac{c_3}{c_2}\, t)}$
$F(x,t)$	$\frac{c_3}{c_2}\left(1 - \sqrt{1 - \frac{2c_2^2}{c_3^2}\, e^{-w(x - \frac{c_3}{c_2}\, t)}}\right)$
Notes	We consider example (a) in Table 6.9 and leave case (b) for future work
Remarks	Future work investigates asymptotic and explicit solutions $c(\lambda, t)$

Table 6.9: General similarity solution for Burgers' eq. with sources: $F_t + F\, F_x = G(x,t)$

Parameters	NEW solution (Example 4.9)
Conditions	$\frac{c_3}{c_2} > 0,\ \ c_3^2 \le 2\, c_2^2$
Definitions	$q = \frac{2c_2^2}{c_3^2}$ and $B = 1 + \sqrt{1 - \frac{c_3^2}{2\, c_2^2}}$
$\lambda\, c_0(\lambda)$	$\begin{cases} \text{given by an inverse Laplace transform of } h(x) \text{ defined as} \\ h(x) = 1 - \sqrt{1 - \frac{2c_2^2}{c_3^2}\, e^{-x}} \end{cases}$
$\lambda\, g(\lambda, t)$	$\delta(\lambda - 1)\, e^{-(Q(t)\, \lambda - \frac{c_3}{c_2}\, t)}$
$Q(t)$	$\begin{cases} 2\, \ln\left(\frac{B^2\, \exp\left(-\frac{c_3}{2\, c_2}\, t\right) + q\, \exp\left(\frac{c_3}{2\, c_2}\, t\right)}{2\, B}\right) + \frac{c_3}{c_2}\, t, & \text{for} \quad t \in [0, T_{gel}) \\ \ln q + \frac{c_3}{c_2}\, t, & \text{for} \quad t \ge T_{gel} \end{cases}$
$c(\lambda, t)$	$\begin{cases} \text{Asymptotic solution as } \lambda \to \infty, \text{ and } \ \forall\, t \ge 0 \\ \frac{c_3}{2\, c_2\, \sqrt{\pi}}\, \lambda^{-5/2}\, e^{-\lambda\, (Q(t) - \frac{c_3}{c_2}\, t - \ln q)} \end{cases}$
T_{gel}	$\frac{c_2}{c_3}\, \ln\left(\frac{B^2}{q}\right)$

Table 6.10: Asymptotic solution for $K(\lambda, \mu, t) = \lambda\, \mu$

6.1.5 $K(\lambda,\mu,t) = (\alpha + \beta\,\lambda)\,(\alpha + \beta\,\mu)$ and $g(\lambda,t) \geq 0$

Parameters	NEW solution (Example 4.11)
Conditions	$a_5 > 0,\ \alpha \in \left(0, \frac{1}{2}\right),\ \beta > 0,\ p \in \left(0, \frac{1}{2\alpha} - 1\right]$
Definitions	$\begin{cases} S(t) = a_5 + \int_0^t e^{-\alpha\,Q(\tau)}\,d\tau \\ A = 1 - \sqrt{1 - 2\,\alpha\,(p+1)} > 0 \end{cases}$
$G(x,t)$	$\frac{2pe^{-\alpha\,Q(t)}}{\alpha^2\,S(t)^2}\left\{\frac{e^{\frac{\alpha}{2\beta}x}}{S(t)^{p+1}} - \alpha\,(p+1) - \sqrt{\left[\frac{e^{\frac{\alpha}{2\beta}x}}{S(t)^{p+1}} - \alpha\,(p+1)\right]^2 - \left[\alpha\,(p+1)\right]^2}\right\}$
$g(\lambda,t)$	given by $\frac{1}{(\alpha+\beta\,\lambda)}\,e^{-(\alpha+\beta\,\lambda)\,Q(t)}\,\mathcal{L}^{-1}\{G(x,t)\}(\lambda,t)$ (numerical)
$Q(t)$	$\frac{\alpha}{2}\,e^{\frac{\alpha}{2}\,Q(t)}\,Q'(t) = \frac{A}{\alpha}\left(\frac{A}{2}\right)^{\frac{1}{p+1}}\left\{1 - \frac{\alpha(p+1)}{A}\,e^{-\frac{\alpha}{2}\,Q(t)}\right\}^{\frac{p}{p+1}}$
$c(\lambda,t)$	$\frac{2\,e^{-(\alpha+\beta\lambda)\,Q(t)}}{(\alpha+\beta\lambda)\,\alpha^{2}\,S(t)}\sum_{k=2}^{\infty}\frac{(2k-2)!}{2^{2k-1}k!(k-1)!}\left[2\alpha(p+1)S(t)^{p+1}\right]^k\,\delta\left(\lambda - \frac{\alpha\,(k-1)}{2\beta}\right)$
Remarks	If $a_5 = 0$ then $c_0(\lambda) = 0$ (no particles at $t = 0$).

Table 6.11: Formal series solution for $K(\lambda,\mu,t) = (\alpha + \beta\,\lambda)\,(\alpha + \beta\,\mu)$

6.1.6 $K(\lambda,\mu)$ general and $g(\lambda,t) = 0$

Parameters	NEW solution
Conditions	c_1, c_2 arbitrary constants
$g(\lambda,t)$	0
$c(\lambda,t)$	$\psi(\lambda)\,(t - \frac{c_2}{c_1})^{-1}$
$\psi(\lambda)$	$\begin{cases} \text{satisfies the IDE} \\ \psi(\lambda) = -\frac{1}{2}\int_0^\lambda K(\lambda-\mu,\mu)\,\psi(\lambda-\mu)\,\psi(\mu)\,d\mu + \psi(\lambda)\int_0^\infty K(\lambda,\mu)\,\psi(\mu)\,d\mu \end{cases}$
Remarks	$\begin{cases} \text{In general, the IDE cannot be solved analytically} \\ \text{Numerical methods need to be employed (future work)} \end{cases}$

Table 6.13: Similarity solutions $c(\lambda,t)$ for a general kernel $K(\lambda,\mu)$ and $g(\lambda,t) = 0$

Parameters	NEW solution (Example 4.10)	Particular solution (Example 4.10)
Conditions	$\mu,\ m > 0,\ \gamma < 0$	If $\mu = 2 \Rightarrow b = \frac{3\alpha}{2\beta},\ \gamma = -\frac{\alpha}{2\beta}$
Definitions	$\gamma = \frac{\alpha - b\beta}{\beta} < 0,\ \ \mu = \frac{2\,b\beta - \alpha}{\alpha} > 1$ and $m = \frac{(-\gamma)^{\mu}}{A_1} > 0$	
$c_0(\lambda)$	$\frac{m}{\alpha+\beta\lambda}\,\delta(\lambda+\gamma)$	$\frac{m}{\alpha+\beta\lambda}\,\delta\left(\lambda - \frac{\alpha}{2\beta}\right)$
$g(\lambda, t)$	0	0
$Q(t)$	$\begin{cases} \frac{2}{\alpha}\ln\left(\frac{2+\alpha\, m\, t}{2}\right), & \text{for } t \in [0, T_{gel}) \\ \frac{1}{b\beta}\ln\left\{\left[\frac{2\,b\,\beta-\alpha}{2(b\beta-\alpha)}\right]^{(2b\beta/\alpha)-1}\left(mb\beta t - \frac{\alpha}{2(b\beta-\alpha)}\right)\right\}, & \text{for } t \geq T_{gel} \end{cases}$	$\begin{cases} \frac{2}{\alpha}\ln\left(\frac{2+\alpha\, m\, t}{2}\right), & \text{for } t \in [0, T_{gel}) \\ \frac{2}{3\alpha}\ln(6\alpha m t - 4), & \text{for } t \geq T_{gel} \end{cases}$
$R(t)$	$\int_0^t e^{-\alpha\, Q(\tau)}\, d\tau$	$\int_0^t e^{-\alpha\, Q(\tau)}\, d\tau$
$c(\lambda, t)$	$\begin{cases} \text{given by the inverse Laplace transf. of } F(x,t) \text{ s.t.} \\ m\left(\frac{\alpha}{2} R(t)\, F(x,t) + 1\right)^{\mu} = F(x,t)\, e^{-\gamma x} \end{cases}$	$\frac{\lambda^{-3/2}\, e^{-(\alpha+\beta\lambda)\, Q(t)}}{(\alpha+\beta\lambda)\,\alpha\, R(t)}\,\sqrt{\frac{2\alpha}{\beta\pi}}\,\left[2\alpha R(t)\, m\right]^{\frac{2\beta}{\alpha}\lambda}$
$M_1(t)$	$\begin{cases} \frac{m(b\,\beta-\alpha)}{b\,\beta^2}, & \text{for } t \in [0, T_{gel}) \\ \frac{m(b\beta-\alpha)(2b\beta-\alpha)}{b\beta^2\left(2(b\beta-\alpha)mb\beta t-\alpha\right)}, & \text{for } t \geq T_{gel} \end{cases}$	$\begin{cases} \frac{m}{3\beta}, & \text{for } t \in [0, T_{gel}) \\ \frac{4\,m}{3\,\beta\,(3\,\alpha\, m\, t-2)}, & \text{for } t \geq T_{gel} \end{cases}$
T_{gel}	$\frac{1}{m\,(b\,\beta-\alpha)}$	$\frac{2}{\alpha\, m}$

Table 6.12: Asymptotic large size ($\lambda \to \infty$) solutions for $K(\lambda, \mu, t) = (\alpha + \beta\,\lambda)\,(\alpha + \beta\,\mu)$

6.2 Future directions

My research in the coagulation theory extends with several other new exciting developments. As part of my future research, I would like to branch out along some of the following lines:

Theoretical work

- *Group symmetry methods for coagulation equations.* I plan to extend the family of source terms proposed in Sections 4.2, 4.3 and obtain more explicit or asymptotic solutions to the coagulation equation. More specifically, I am interested in extending the symmetry method in Section 4.3 such that we include a more general, non-negative function $\varphi(s)$, not necessarily depending on the similarity profile $\psi(s)$, and thus extend the family of source functions $g(\lambda, t)$.

- *Inverse Laplace transforms. Contour integration.* In Section 4.2, we expressed the explicit solutions as formal series. My plan is to make use of the contour integration in order to obtain the inverse Laplace Transform and if possible to derive explicit solutions to the coagulation equation.

- *Group symmetry methods for coagulation-fragmentation equations with diffusion.* Elhanbaly [9] investigated the existence of similarity solutions for fragmentation equations with mass loss. In my future research, I plan to extend the symmetry group analysis I proposed for the coagulation equations in order to derive new similarity solutions to the coagulation-fragmentation equation. Then, I intend to apply this study for the case when both coagulation, fragmentation, and diffusion processes are present in the system.

- *Gelation phenomena: gel-time.* I intend to investigate the gelation phenomena in the case when both coagulation, fragmentation and diffusion occur. I want to compare the gel-times in these systems with the corresponding times in the case when only coagulation is present. It is also interesting to provide (whenever possible) some explicit formulas for the gel-time, or some estimates (lower/upper bounds).

- *Total mass of particles.* Shirvani and van Roessel [89] have provided an explicit formula for the total mass $M_1(t)$ for all time for a coagulation kernel $K(\lambda, \mu) =$

$(\alpha + \beta\,\lambda)\,(\alpha + \beta\,\mu)$. I plan to pursue a similar analysis to obtain a general post-gelation formula for the first moment in the case when particle sources/sinks are present in the system for a bilinear, separable time-dependent kernel $K(\lambda, \mu, t)$.

Numerical work

- *Stability and error analysis.* - Kumar et al [60] were the first to develop numerical algorithms based on moving mesh techniques and refining the grid based on preservation of two properties of the distribution. In my future work, I plan to extend these methods to the case of coagulation or coagulation-fragmentation equations with particle sources and sinks without imposing such restrictions. I also intend to investigate some ways of choosing the maximum particle size X_{max} and other approximations for the convolution integral, such as Fast Fourier Transforms.

  - Sandu et al [90] suggest the use of spectral methods. I plan to apply these methods to the unbounded kernels in Section 5.2.

  - Another direct approach to solve the coagulation equation (5.2) is to discretize the system first in time and then in size. In this way, the time integration leads to a linear Fredholm integral equation of second kind for the distribution function $c(x, t^{k+1})$ (see e.g. [90]).

  - Develop new numerical methods for time-dependent kernels $K(\lambda, \mu, t)$ as presented in Section 4.3.

- *New classes of efficient stochastic algorithms.* Wagner [14] proposed some classes of stochastic algorithms for coagulation equations (without sources and sinks). As another long-term goal, I would like to investigate some new classes of efficient stochastic algorithms for the numerical treatment of these coagulation-fragmentation equations with diffusion. This stochastic approach seems to evolve as a possible avenue for new research in the future. I also plan to extend the mass-flow algorithms to these general equations.

- *Gelation phenomena: gel-time.* I intend to investigate better ways of determining the numerical onset of gelation phenomena in the case when both coagulation, fragmentation and diffusion occur.

- *Numerical inversion of Laplace transforms.* I propose a numerical method that determines the numerical solution by first solving the quasilinear associated

PDE (4.10) combined with a numerical inversion of the vector of discrete solutions.

Chapter 7

Appendix

7.1 Proofs of some theorems in Chapter 4.2

Optimal system of one-dimensional subalgebras of (4.34).

Proof of Theorem 4.1:
Indeed, consider the following vector field from the Lie algebra L_8

$$V = a_8\, V_8 + a_7\, V_7 + a_6\, V_6 + a_5\, V_5 + a_4\, V_4 + a_3\, V_3 + a_2\, V_2 + a_1\, V_1,$$

where $a_1, a_2, \cdots, a_8$ are arbitrary constants. Our task is to simplify V, and so its coefficients as much as possible. This can be done by judiciously applying adjoint maps to it (see [80] for details).

Case A. Let' s assume first that $a_8 \neq 0$. One can scale V, if necessary and assume that $a_8 = 1$. By acting on the vector V by the adjoint operation $V' = Ad(\exp(\varepsilon\, V_2))V$ we obtain the following relation

$$\begin{aligned} V' = V_8 + (a_7 - \varepsilon)\, V_7 + a_6 V_6 + a_5 V_5 + (a_4 - \varepsilon\, a_6)\, V_4 + (a_3 - 2\varepsilon\, a_6)\, V_3 \\ + (a_2 - \varepsilon\, a_3)\, V_2 + (a_1 - \varepsilon\, a_5)\, V_1 \end{aligned} \tag{7.1}$$

From (7.1), we can eliminate the coefficient of V_7 by taking the value of the group parameter $\varepsilon = a_7$. Then we have

$$V' = V_8 + a_6 V_6 + a_5 V_5 + a_4'\, V_4 + a_3'\, V_3 + a_2'\, V_2 + a_1'\, V_1,$$

where a_4', a_3', a_2', a_1' are new arbitrary constants (depending on a_4, a_3, a_2, a_1). Next, we act on V' by $Ad(\exp((a_4'/2)\, V_1))$ to cancel the coefficient of V_4, leading to

$$V'' = V_8 + a_6 V_6 + a_5' V_5 + a_3' V_3 + a_2' V_2 + a_1' V_1.$$

Finally, if we act on V'' by $Ad(\exp(a_6 V_5))$ we can make the coefficient of V_6 vanish and obtain

$$\tilde{V} = V_8 + a_5' V_5 + a_3' V_3 + a_2' V_2 + a_1' V_1$$

We have a few cases to consider here:

A1. If $a_5' = 0$ and $a_3' \neq 0$ or $a_3' = 0$ and $a_5' \neq 0$ then the vector form $\tilde{V}$ cannot be simplified further, and we obtain the vector fields $\tilde{V} = V_8 + V_5 + a_2' V_2 + a_1' V_1$, and $V_8 + V_5 + a_2' V_2 + a_1' V_1$, where $a_1', a_2' \in \mathbb{R}$.

A2. If $a_5' = a_3' = 0$ then we can act on $\tilde{V}$ by $Ad(\exp(\varepsilon V_7))$ which gives

$$\tilde{V} = V_8 + a_1' V_1 + (a_2' + \varepsilon a_1') V_2.$$

For $\tilde{V}$, if $a_1' \neq 0$ then we can eliminate the coefficient of V_2 by choosing the parameter $\varepsilon = -a_2'/a_1'$ and obtain $\tilde{V} = V_8 + a_1' V_1$, $a_1' \in \mathbb{R} \setminus \{0\}$. On the other hand, if $a_1' = 0$ then we have $\tilde{V} = V_8 + a_2' V_2$, where $a_2' \in \mathbb{R}$.

Thus, we obtain that every one-dimensional subalgebra generated by a vector field V with $a_8 \neq 0$ is equivalent to a subalgebra spanned by the vector fields $V_8 + V_5 + a_2 V_2 + a_1 V_1$, $V_8 + V_3 + a_2 V_2 + a_1 V_1$, $V_8 + V_1$, $V_8 - V_1$, $V_8 + a_2 V_2$, where $a_1, a_2 \in \mathbb{R}$.

Case B. The remaining one-dimensional subalgebras are spanned by vectors of the form above with $a_8 = 0, a_7 \neq 0$. Take the following vector field

$$V = V_7 + a_6 V_6 + a_5 V_5 + a_4 V_4 + a_3 V_3 + a_2 V_2 + a_1 V_1 \tag{7.2}$$

In (7.2), acting on V by $Ad(\exp(a_2 V_1))$ and $Ad(\exp(a_3 V_5))$ we obtain

$$V'' = V_7 + a_6 V_6 + a_5 V_5 + a_4 V_4 + a_1 V_1$$

We need to consider the following subcases:

B1. If $a_6 = 0$ then acting on $V'' = V_7 + a_5 V_5 + a_4 V_4 + a_1 V_1$ by $Ad(\exp(\varepsilon V_2))$ we get $\tilde{V} = V_7 + a_5 V_5 + (a_1 - \varepsilon a_5) V_1 + a_4 V_4$. We have two subcases to consider:

(a) If $a_5 \neq 0$ then we can choose $\varepsilon = a_1/a_5$ and make the coefficient of V_1 disappear. Then $\tilde{V} = V_7 + V_5 + a_4 V_4$, where $a_4 \in \mathbb{R}$.

(b) If $a_5 = 0$ then we get $\tilde{V} = V_7 + a_4 V_4 + a_1 V_1$, where $a_1, a_4 \in \mathbb{R}$.

B2. If $a_5 = 0$ and $a_6 \neq 0$ then we get $V'' = V_7 + V_6 + a_4 V_4 + a_1 V_1$, where $a_1, a_4 \in \mathbb{R}$.

Therefore, every one-dimensional subalgebra generated by a vector field V with $a_8 = 0$ and $a_7 \neq 0$ is equivalent to a subalgebra spanned by either $V_7 + V_5 + a_4 V_4$, $V_7 + a_4 V_4 + a_1 V_1$, or $V_7 + V_6 + a_4 V_4 + a_1 V_1$, where $a_1, a_4 \in \mathbb{R}$.

Case C. The remaining one-dimensional subalgebras are spanned by vectors of the form above with $a_8 = a_7 = 0$, $a_6 \neq 0$. In this case, we first rescale V to get $a_6 = 1$ and acting on V above by $Ad(\exp(a_5 V_1))$, $Ad(\exp(a_4 V_2))$, we obtain

$$V' = V_6 + a_3 V_3 + a_2 V_2 + a_1 V_1$$

A few subcases are included below:

C1. If $a_3 = 0$ then acting on the new V' by $Ad(\exp(\varepsilon V_5))$ we get $\tilde{V} = V_6 + a_2 V_2 + (a_1 + \varepsilon a_2) V_1$. We have two subcases to consider

(a) If $a_2 \neq 0$ then we can choose $\varepsilon = -a_1/a_2$ and make the coefficient of V_1 disappear and thus we get the new vector form $V'' = V_6 + a_2 V_2$, where $a_2 \in \mathbb{R}$.

(b) If $a_2 = 0$ then we obtain $V'' = V_6 + a_1 V_1$, where $a_1 \in \mathbb{R}$.

C2. If $a_3 \neq 0$ then we get $V'' = V_6 + V_3 + a_2 V_2 + a_1 V_1$, where $a_1, a_2 \in \mathbb{R}$.

Thus, every one-dimensional subalgebra generated by a vector field V with $a_8 = a_7 = 0$ and $a_6 \neq 0$ is equivalent to a subalgebra spanned by either $V_6 + V_3 + a_2 V_2 + a_1 V_1$, $V_6 + a_1 V_1$, or $V_6 + a_2 V_2$, where $a_1, a_2 \in \mathbb{R}$.

Case D. The remaining one-dimensional subalgebras are spanned by vectors of the form above with $a_8 = a_7 = a_6 = 0, a_5 \neq 0$. In this case, by acting on V above by $Ad(\exp(a_1 V_1))$ we obtain

$$V' = V_5 + a_4 V_4 + a_3 V_3 + a_2 V_2$$

If $a_4 = 0$ then we have $\tilde{V} = V_5 + a_3 V_3 + a_2 V_2$, with $a_2, a_3 \in \mathbb{R}$. On the other hand, if $a_4 \neq 0$ then the new vector form becomes $V'' = V_5 + V_4 + a_3 V_3 + a_2 V_2$, where $a_2, a_3 \in \mathbb{R}$. Hence, every one-dimensional subalgebra generated by a vector field V with $a_8 = a_7 = a_6 = 0$ and $a_5 \neq 0$ is equivalent to a subalgebra spanned by either $V_5 + a_3 V_3 + a_2 V_2$ or $V_5 + V_4 + a_3 V_3 + a_2 V_2$, with $a_2, a_3 \in \mathbb{R}$.

Case E. The remaining one-dimensional subalgebras are spanned by vectors of the form above with $a_8 = a_7 = a_6 = a_5 = 0, a_4 \neq 0.$ In this case, by acting on V above by $Ad(\exp(\varepsilon\, V_2))$ we obtain

$$V' = V_4 + a_3\, V_3 + (a_2 - \varepsilon\, a_3)\, V_2 + a_1\, V_1$$

If $a_3 \neq 0$ then we can choose $\varepsilon = a_2/a_3$ to make the coefficient of V_2 disappear and we get $\bar{V} = V_4 + V_3 + a_1\, V_1$, with $a_1 \in \mathbb{R}$. On the other hand, if $a_3 = 0$ then the new vector form becomes $V'' = V_4 + a_2\, V_2 + a_1\, V_1$, where $a_2, a_1 \in \mathbb{R}$. So, every one-dimensional subalgebra generated by a vector field V with $a_8 = a_7 = a_6 = a_5 = 0$ and $a_4 \neq 0$ is equivalent to a subalgebra spanned by either $V_4 + a_3\, V_3 + a_2\, V_2$, $V_4 + a_2\, V_2$, or $V_4 + a_3\, V_3$, with $a_2, a_3 \in \mathbb{R}$.

Case F. The remaining one-dimensional subalgebras are spanned by vectors of the form above with $a_8 = a_7 = a_6 = a_5 = a_4 = 0, a_3 \neq 0$. In this case, by acting on V above by $Ad(\exp(a_2\, V_2))$ we obtain $V' = V_3 + a_1\, V_1$, where $a_1 \in \mathbb{R}$. Similarly, we have two more one-dimensional subalgebras $V_2 + a_1\, V_1$ and $V = V_1$, with $a_1 \in \mathbb{R}$ and the proof of Theorem 4.1 is now complete. ☐

Optimal system of one-dimensional subalgebras of (4.101).

Proof of Theorem 4.4:
Indeed, take the following vector field from the Lie algebra $\mathcal{L}_8$

$$V = c_8\, V_8 + c_7\, V_7 + c_6\, V_6 + c_5\, V_5 + c_4\, V_4 + c_3\, V_3 + c_2\, V_2 + c_1\, V_1,$$

where $c_1, c_2, ..., c_8$ are arbitrary constants. Similar to the previous case, our task is to simplify V as much as possible by applying adjoint maps to it (see [80] for a details).

Case A. Let' s assume first that $c_8 \neq 0$. One can rescale V, if necessary, and assume that $c_8 = 1$. By acting on V by the adjoint operation $V' = Ad(\exp(\varepsilon\, V_6))V$ we obtain the following vector field

$$\begin{aligned} V' = V_8 + \Big(c_7 - \varepsilon\,\frac{\alpha}{2\,\beta}\Big)\, V_7 + \Big(c_6 - \varepsilon\,\frac{\alpha}{\beta}\, c_5\Big)\, V_6 + (c_5 + \varepsilon\, c_2)\, V_5 + \Big(c_4 - \varepsilon\,\frac{\alpha}{2\,\beta}\, c_3\Big)\, V_4 \\ + c_3\, V_3 + c_2\, V_2 + c_1\, V_1 \end{aligned} \tag{7.3}$$

It follows from (7.3), that we can eliminate the coefficient of V_7 by choosing the value of the group parameter $\varepsilon = \frac{2\beta c_7}{\alpha}$. Then we have

$$V' = V_8 + c_6' V_6 + c_5' V_5 + c_4' V_4 + c_3 V_3 + c_2 V_2 + c_1 V_1,$$

where c_6', c_5', c_4' are new arbitrary constants depending on the previous constants. Next, if we act on V' by $Ad(\exp(\varepsilon V_2))$ we obtain the vector field

$$V'' = V_8 + c_6' V_6 + (c_5' - \varepsilon c_6') V_5 + c_4' V_4 + (c_3 - \varepsilon c_4') V_3 + \left(c_2 - \varepsilon c_1 + \varepsilon \frac{\alpha}{\beta} c_5'\right) V_2 + c_1 V_1. \quad (7.4)$$

We consider next two separate cases:

Case A1: If $c_6' \neq 0$ (we can rescale V'' such that $c_6' = 1$), then we can make the coefficient of V_5 in (7.4) vanish by choosing $\varepsilon = c_5'/c_6'$ and obtain $V''' = V_8 + V_6 + c_4' V_4 + c_3' V_3 + c_2' V_2 + c_1 V_1$. Next, we can make the coefficient of V_4 in V''' disappear by acting on V''' by $Ad(\exp(-\frac{2\beta c_4'}{\alpha} V_3))$ and obtain the vector field $\hat{V} = V_8 + V_6 + c_3' V_3 + c_2^* V_2 + c_1 V_1$, which cannot be simplified further.

Case A2: If $c_6' = 0$, then we obtain

$$V'' = V_8 + c_5' V_5 + c_4' V_4 + (c_3 - \varepsilon c_4') V_3 + \left(c_2 - \varepsilon c_1 + \varepsilon \frac{\alpha}{\beta} c_5'\right) V_2 + c_1 V_1. \quad (7.5)$$

(a) If in (7.5), we have $c_4' \neq 0$, then we can choose $\varepsilon = c_3/c_4'$ to make the coefficient of V_3 vanish and by rescaling V'' we set $c_4' = 1$, so we get

$$V''' = V_8 + V_4 + c_5' V_5 + c_2' V_2 + c_1 V_1$$

If we apply on V''' the adjoint operation $Ad(\exp(\varepsilon V_8))$ and choose $\varepsilon \neq 1/(c_1 - c_5'\alpha/(2\beta))$, we can rescale V''' so that the coefficient of V_8 equals to one. Next, set $\varepsilon = \alpha c_5'/2$ and obtain $V^* = V_8 + V_4 + c_1^* V_1 + c_2^* V_2$. Finally, on V^* apply $Ad(\exp(-c_2^* \beta) V_3)$ to obtain $V_8 + V_4 + c_1^* V_1$, where $c_1^* \in \mathbb{R}$, with no possible further reduction.
(b) If in (7.5), we have $c_4' \neq 0$, then acting on V'' by $Ad(\exp(\varepsilon V_3))$ we get

$$\tilde{V} = V_8 + c_5' V_5 + \left(c_3 + \varepsilon c_5' \frac{\alpha}{2\beta}\right) V_3 + \left(c_2' + \frac{\varepsilon}{\beta}\right) V_2 + c_1 V_1 \quad (7.6)$$

(b1) Assume that $c_5' \neq 0$ then we can make the coefficient of V_3 in $\tilde{V}$ disappear if we choose $\varepsilon = -\frac{2\beta c_3}{c_5' \alpha}$, By rescaling $\tilde{V}$ s.t. $c_5' = 1$ we obtain $V'''' = V_8 + V_5 + c_2 V_2 + c_1 V_1$. Next, act on V'''' by $Ad(\exp(\varepsilon V_2))$ to get

$$V^{**} = V_8 + V_5 + \left[c_2 + \varepsilon \left(\frac{\alpha}{\beta} - c_1\right)\right] V_2 + c_1 V_1$$

Two subcases arise here, if $c_1 \neq \frac{\alpha}{\beta}$ then we get $V^{**} = V_8 + V_5 + c_1 V_1$, or if $c_1 = \frac{\alpha}{\beta}$ then we have $V^{**} = V_8 + V_5 + \frac{\alpha}{\beta} V_1 + c_2 V_2$, where $c_2 \in \mathbb{R}$.

(b2) If $c'_5 = 0$ then we can act on $\tilde{V}$ in (7.6) by $Ad(\exp(-c'_2 \beta) V_3)$ to obtain

$$V'''' = V_8 + c_3 V_3 + c_1 V_1$$

whose coefficients can't be simplified further.

Therefore every one-dimensional subalgebra generated by a vector field V with $c_8 \neq 0$ is equivalent to a subalgebra spanned by the following vector fields $V_8 + V_6 + c_3 V_3 + c_2 V_2 + c_1 V_1$; $V_8 + V_4 + c_1 V_1$; $V_8 + c_3 V_3 + c_1 V_1$, where $c_3, c_5, c_2, c_1 \in \mathbb{R}$, or $V_8 + V_5 + c_1 V_1$, (where $c_1 \neq \frac{\alpha}{\beta}$) and $V_8 + V_5 + \frac{\alpha}{\beta} V_1 + c_2 V_2$, where $c_2 \in \mathbb{R}$.

Case B. The remaining one-dimensional subalgebras are spanned by vectors with $c_8 = 0, c_7 \neq 0$ of the form

$$V = V_7 + c_6 V_6 + c_5 V_5 + c_4 V_4 + c_3 V_3 + c_2 V_2 + c_1 V_1. \tag{7.7}$$

In (7.7), acting by $Ad(\exp(\varepsilon V_6))$, we obtain

$$V' = V_7 + \left(c_6 + \varepsilon c_1 - \varepsilon \frac{\alpha}{\beta} c_5\right) V_6 + (c_5 + \varepsilon c_2) V_5 + \left(c_4 - \varepsilon \frac{\alpha}{2\beta} c_3\right) V_4 + c_3 V_3 + c_2 V_2 + c_1 V_1 \tag{7.8}$$

Next, we consider two separate cases:

Case B1: If $c_2 \neq 0$ then we can eliminate the coefficient of V_5 in (7.8) by setting $\varepsilon = -c_5/c_2$, and rescale V' s.t. $c_2 = 1$ to get

$$V' = V_7 + V_2 + c'_6 V_6 + c'_4 V_4 + c_3 V_3 + c_1 V_1.$$

By acting on V' by $Ad(\exp(\varepsilon V_4))$ we have

$$V'' = V_7 + V_2 + \left(c'_6 - \varepsilon \frac{2}{\alpha}\right) V_6 + (c'_4 + \varepsilon c_1) V_4 + (c_3 + \varepsilon) V_3 + c_1 V_1 \tag{7.9}$$

In (7.9), if $c_1 \neq 0$, then choosing $\varepsilon = -c'_4/c_1$, we can make the coefficient of V_4 vanish and obtain $V''' = V_7 + V_2 + V_1 + c'_6 V_6 + c'_3 V_3$, which cannot be simplified further by taking any adjoint operations on V'''. However, if $c_1 = 0$ in (7.9) then we obtain $V''' = V_7 + V_2 + c'_6 V_6 + c'_4 V_4 + c'_3 V_3$, and acting on the latter by $Ad(\exp(\frac{\alpha c'_6}{2} V_4))$ yields $V'''' = V_7 + V_2 + c'_4 V_4 + c'_3 V_3$.

Case B2: If in (7.8), $c_2 = 0$ then acting on V by $Ad(\exp(\varepsilon\, V_4))$ we have

$$V'' = V_7 + \left(c_6' - \varepsilon\,\frac{2}{\alpha}\right) V_6 + c_5\, V_5 + \left(c_4' + \varepsilon\, c_1 - \varepsilon\,\frac{\alpha}{2\,\beta}\, c_5\right) V_4 + c_3\, V_3 + c_1\, V_1.$$

If $c_1 \neq \frac{\alpha\, c_5}{2\beta}$ then set $\varepsilon = -\frac{c_4'}{c_1 - \alpha\, c_5/(2\,\beta)}$ to get $V''' = V_7 + c_6'\, V_6 + c_5\, V_5 + c_3\, V_3 + c_1\, V_1$. Moreover, by acting on V''' by $Ad(\exp(\varepsilon\, V_7))$, where we assume $\varepsilon \neq \frac{2\beta}{\alpha\, c_5}$, and rescaling the new vector s.t. the coefficient of V_7 equals to one, we have

$$V'''' = V_7 + c_6''\, V_6 + \left(c_5' + \varepsilon\,\frac{4}{\alpha}\, c_3'\right) + c_3'\, V_3 + \left(c_1' + \varepsilon\,\frac{3\, c_3'}{\beta}\right) V_1. \tag{7.10}$$

In (7.10), if $c_3' \neq 0$, then we can set $\varepsilon = -\frac{c_1'\,\beta}{3\, c_3'}$ to obtain $V^* = V_7 + V_3 + c_6^*\, V_6 + c_5^*\, V_5$. On the other hand, if in (7.10) we have $c_3' = 0$ then we set $\varepsilon = -\frac{\beta\, c_1'}{3}$ and obtain

$$\bar{V} = V_7 + c_6^*\, V_6 + c_5^*\, V_5 + c_1^*\, V_1.$$

Furthermore, acting on $\bar{V}$ by $Ad(\exp(\varepsilon\, V_6))$ and assuming $c_1^* \neq \frac{\alpha\, c_5^*}{\beta}$ one obtains

$$\tilde{V} = V_7 + \bar{c}_5\, V_5 + \bar{c}_1\, V_1,$$

which cannot be simplified further. Thus, every one-dimensional subalgebra generated by a vector field V with $c_8 = 0$ and $c_7 \neq 0$ is equivalent to a subalgebra spanned by $V_7 + V_2 + c_4\, V_4 + c_3\, V_3$, $V_7 + V_2 + V_1 + c_6\, V_6 + c_3\, V_3$, $V_7 + c_5\, V_5 + c_1\, V_1$, and $V_7 + V_3 + c_6\, V_6 + c_5\, V_5$, where $c_1, c_3, c_4, c_5, c_6 \in \mathbb{R}$.

Case C. The remaining one-dimensional subalgebras are spanned by vectors with $c_8 = c_7 = 0, c_6 \neq 0$ of the form

$$V = V_6 + c_5\, V_5 + c_4\, V_4 + c_3\, V_3 + c_2\, V_2 + c_1\, V_1. \tag{7.11}$$

In (7.11), acting by $Ad(\exp(\varepsilon\, V_4))$, we obtain

$$V' = V_6 + c_5\, V_5 + \left(c_4 + \varepsilon\, c_1 - \varepsilon\frac{\alpha}{2\,\beta}\, c_5\right) V_4 + (c_3 + \varepsilon\, c_2)\, V_3 + c_2\, V_2 + c_1\, V_1 \tag{7.12}$$

Next, we consider two separate cases:

Case C1: If $c_2 \neq 0$ then choose $\varepsilon = -c_3/c_2$ in (7.12). Next, apply $Ad(\exp(-c_5\, V_6))$ on V' to eliminate the coefficients of V_3, and V_5, respectively. We obtain

$$V'' = V_6 + V_2 + c_4'\, V_4 + c_1\, V_1$$

Next, by acting on V'' by $Ad(\exp(-\frac{2\beta c_4'}{\alpha} V_3))$ we get $V''' = V_6 + V_2 + c_1 V_1$, where $c_1 \in \mathbb{R}$.

Case C2: If $c_2 = 0$ in (7.12) then acting on V' by $Ad(\exp(\varepsilon V_3))$ we get

$$V'''' = V_6 + c_5 V_5 + \left(c_4' + \varepsilon \frac{\alpha}{2\beta}\right) V_4 + \left(c_3 + \varepsilon \frac{\alpha}{2\beta} c_5\right) V_3 + c_1 V_1$$

There are two subcases to consider for V'''':

(i) If $c_5 = 0$ then we have $V'''' = V_6 + c_4' V_4 + c_3 V_3 + c_1 V_1$, and applying $Ad(\exp(\varepsilon V_4))$ we obtain

$$\bar{V} = V_6 + (c_4' + \varepsilon c_1) V_4 + c_3 V_3 + c_1 V_1 \tag{7.13}$$

In this case, if $c_1 = 0$ then acting on $\bar{V}$ by $Ad(\exp(-\frac{2\beta c_4}{\alpha}))$ we get $V_6 + c_3 V_3$. On the other hand, if $c_1 \neq 0$ then choose $\varepsilon = -c_4'/c_1$ in (7.13) to obtain $V_6 + V_1 + c_3 V_3$, where for both vectors obtained above we have $c_3 \in \mathbb{R}$.

(ii) If in (7.12), we have $c_5 \neq 0$ then choose $\varepsilon = -\frac{2\beta c_3}{\alpha}$ and obtain $V^* = V_6 + V_5 + c_4'' V_4 c_1 V_1$, and applying on V^* the adjoint operation $Ad(\exp(\varepsilon V_4))$ we obtain

$$V^{**} = V_6 + V_5 + \left[c_4'' + \varepsilon \left(c_1 - \frac{\alpha}{2\beta}\right)\right] V_4 + c_1 V_1.$$

In this case, if $c_1 = \frac{\alpha}{2\beta}$ then we get $\hat{V} = V_6 + V_5 + \frac{\alpha}{2\beta} V_1 + c_4 V_4$, where $c_4 \in \mathbb{R}$. On the other hand, if $c_1 \neq \frac{\alpha}{2\beta}$ then choose $\varepsilon = \frac{c_4''}{-c_1+\alpha/(2\beta)}$ to get

$$\tilde{V} = V_6 + V_5 + c_1 V_1, \quad \text{where} \quad c_1 \in RR, \quad \text{and} \quad c_1 \neq \frac{\alpha}{2\beta}$$

Thus, we obtain that every one-dimensional subalgebra generated by a vector field V with $c_8 = c_7 = 0$ and $c_6 \neq 0$ is equivalent to a subalgebra spanned by either $V_6 + V_2 + c_1 V_1$, $V_6 + c_3 V_3$, $V_6 + V_1 + c_3 V_3$, $V_6 + V_5 + \frac{\alpha}{2\beta} V_1 + c_4 V_4$, where $c_1, c_3, c_4 \in \mathbb{R}$ and $V_6 + V_5 + c_1 V_1$, where $c_1 \neq \frac{\alpha}{2\beta}$.

Case D. The remaining one-dimensional subalgebras are spanned by vectors with $c_8 = c_7 = c_6 = 0, c_5 \neq 0$ of the form

$$V = V_5 + c_4 V_4 + c_3 V_3 + c_2 V_2 + c_1 V_1. \tag{7.14}$$

In (7.14), acting by $Ad(\exp(\varepsilon V_4))$, we obtain

$$V' = V_5 + \left(c_4 + \varepsilon c_1 - \varepsilon \frac{\alpha}{2\beta}\right) V_4 + (c_3 + \varepsilon c_2) V_3 + c_2 V_2 + c_1 V_1 \tag{7.15}$$

Next, we consider two separate cases:

Case D1: If $c_1 \neq \frac{\alpha}{2\beta}$ then we choose $\varepsilon = -\frac{c_4}{c_1 - \frac{\alpha}{2\beta}}$ in (7.15) and obtain

$$V'' = V_5 + c_3' V_3 + c_2 V_2 + c_1 V_1$$

Next, act on V'' by $Ad(\exp(\varepsilon V_2))$ to obtain

$$V'' = V_5 + c_3' V_3 + \left(c_2 - \varepsilon c_1 + \varepsilon \frac{\alpha}{\beta}\right) V_2 + c_1 V_1 \tag{7.16}$$

Then there are two subcases to consider for (7.16):
(a) If $c_1 \neq \frac{\alpha}{\beta}$ then set $\varepsilon = -\frac{c_2}{\frac{\alpha}{\beta} - c_1}$ in (7.16) to eliminate the coefficient of V_2 and then apply $Ad(\exp(-\frac{2\beta c_3'}{\alpha} V_3))$ to eliminate the coefficient of V_3. We obtain $V''' = V_5 + c_1 V_1$, where c_1 any constant s.t. $c_1 \neq \frac{\alpha}{\beta}, \frac{\alpha}{2\beta}$.

(b) If $c_1 = \frac{\alpha}{\beta}$, then V'' in (7.16) becomes $V'''' = V_5 + \frac{\alpha}{\beta} V_1 + c_3' V_3 + c_2 V_2$. Acting on V'''' by $Ad(\exp(-\frac{2\beta c_3'}{\alpha} V_3))$ then we get the vector field

$$\hat{V} = V_5 + \frac{\alpha}{\beta} V_1 + c_2 V_2 \quad \text{where } c_2 \in \mathbb{R}$$

Case D2: If $c_1 = \frac{\alpha}{2\beta}$ then (7.15) becomes

$$\bar{V} = V_5 + \frac{\alpha}{2\beta} V_1 + c_4 V_4 + c_3' V_3 + c_2 V_2 \tag{7.17}$$

and applying $Ad(\exp(-\frac{2\beta c_2}{\alpha} V_2))$ to eliminate the coefficient of V_2 we get

$$V^* = V_5 + \frac{\alpha}{2\beta} V_1 + c_4 V_4 + c_3' V_3$$

Finally, acting on V^* by $Ad(\exp(-\frac{2\beta c_3'}{\alpha} V_3))$ we can eliminate the coefficient of V_3 and obtain the vector field

$$\mathcal{V} = V_5 + \frac{\alpha}{2\beta} V_1 + c_4 V_4 \quad \text{where } c_4 \in \mathbb{R}$$

which can't be simplified further. Hence, every one-dimensional subalgebra generated by a vector field V with $c_8 = c_7 = c_6 = 0$ and $c_5 \neq 0$ is equivalent to a subalgebra spanned by $V_5 + c_1 V_1$, where c_1 is any arbitrary constant and $c_1 \neq \frac{\alpha}{\beta}, \frac{\alpha}{2\beta}$, and $V_5 + \frac{\alpha}{\beta} V_1 + c_2 V_2$ where $c_2 \in \mathbb{R}$.

Case E. The remaining one-dimensional subalgebras are spanned by vectors with $c_8 = c_7 = c_6 = c_5 = 0, c_4 \neq 0$ of the form

$$V = V_4 + c_3 V_3 + c_2 V_2 + c_1 V_1. \tag{7.18}$$

In (7.18), acting by $Ad(\exp(\varepsilon V_2))$, we obtain

$$V' = V_4 + (c_3 - \varepsilon) V_3 + (c_2 - \varepsilon c_1) V_2 + c_1 V_1 \tag{7.19}$$

Next, we consider two separate cases:

Case E1: If $c_1 \neq 0$ then we choose $\varepsilon = \frac{c_2}{c_1}$ in (7.19) and obtain $V'' = V_4 + V_1 + c_3' V_3 + c_2' V_2$. By acting on V'' by $Ad(\exp(c_3' V_2))$, we get the vector field $V^* = V_4 + V_1 + c_2^* V_2$, where $c_2^* \in \mathbb{R}$.

Case E2: If $c_1 = 0$ in (7.19) then we obtain $\bar{V} = V_4 + c_3' V_3 + c_2 V_2$, and acting on $\bar{V}$ by $Ad(\exp(\varepsilon V_4))$ we obtain

$$V''' = V_4 + (c_3' + \varepsilon c_2) V_3 + c_2 V_2 \tag{7.20}$$

In this case, if $c_2 \neq 0$ then set $\varepsilon = -\frac{c_3'}{c_2}$ to make the coefficient of V_3 vanish and thus we have $\hat{V} = V_4 + c_2 V_2$, where $c_2 \in \mathbb{R} \setminus \{0\}$. On the other hand, if in (7.20) we have $c_2 = 0$ then we can apply $Ad(\exp(c_3' V_2))$ and thus obtain V_4. Therefore, every one-dimensional subalgebra generated by a vector field V with $c_8 = c_7 = c_6 = c_5 = 0$ and $c_4 \neq 0$ is equivalent to a subalgebra spanned by either $V_4 + V_1 + c_2 V_2$, and $V_4 + c_2 V_2$ where $c_2 \in \mathbb{R}$.

Case F. The remaining one-dimensional subalgebras are spanned by vectors of the form $V = V_3 + c_2 V_2 + c_1 V_1$, with $c_8 = c_7 = c_6 = c_5 = c_4 = 0$, $c_3 \neq 0$. In this case, by acting on V above by $Ad(\exp(\varepsilon V_2))$ we obtain

$$V' = V_3 + (c_2 - \varepsilon c_1) V_2 + c_1 V_1$$

In this case, if $c_1 \neq 0$ then we can make the coefficient of V_2 disappear by choosing $\varepsilon = \frac{c_2}{c_1}$ and thus obtain the vector field $\mathcal{V} = V_3 + c_1 V_1$, where $c_1 \in \mathbb{R} \setminus \{0\}$.

Moreover, if $c_1 = 0$ then we get $V_3 + c_2 V_2$, where $c_2 \in \mathbb{R}$. Hence, every one-dimensional subalgebra generated by a vector field V with $c_8 = c_7 = c_6 = c_5 = c_4 = 0$ and $c_3 \neq 0$ is equivalent to a subalgebra spanned by either $V_3 + c_2 V_2$, and $V_3 \pm V_1$ where $c_2 \in \mathbb{R}$. Similarly, we obtain two more one-dimensional subalgebras spanned by the vector fields $V_2 + c_1 V_1$ and $V = V_1$, where $c_1 \in \mathbb{R}$. Thus the proof of Theorem 4.4 is now complete. □

Optimal system of one-dimensional subalgebras of (4.136)

Proof of Theorem 4.5:
Indeed, let's consider the following vector field from the Lie algebra $\mathcal{L}_4$

$$v = a_1\, V_1 + a_2\, V_2 + a_4\, V_3 + a_5\, V_4,$$

where a_1, a_2, a_4, a_5 are arbitrary constants. Our task again is to simplify v, and its coefficients as much as possble by judiciously applying adjoint maps to v.

Let's assume first that $a_1 \neq 0$. One can scale v, if necessary and assume that $a_1 = 1$. By acting on the vector $v = V_1 + a_2\, V_2 + a_4\, V_3 + a_5\, V_4$ by the adjoint operation $v' = Ad(\exp(\varepsilon\, V_4))$ we obtain the following new vector field

$$v' = V_1 + a_2\, V_2 + a_4\, V_3 + \left[a_5 - \varepsilon\left(1 - \frac{2\,a_4}{\beta}\right)\right] V_4$$

If $a_4 \neq \frac{\beta}{2}$ then we can set $\varepsilon = \frac{a_5}{1 - \frac{2\,a_4}{\beta}}$ to eliminate the coefficient of V_4 and thus we obtain the new vector field $v'' = V_1 + a_2\, V_2 + a_4\, V_3$, where a_2 is arbitrary, whose coefficients cannot be reduced further. On the other hand, if $a_4 = \frac{\beta}{2}$ then we obtain $\bar{v} = V_1 + \frac{\beta}{2}\, V_3 + a_2\, V_2 + a_5\, V_4$, which cannot be simplified further. Therefore (i) is proved.

The remaining one-dimensional subalgebras are spanned by vectors with $a_1 = 0$ and $a_2 \neq 0$. Take the following vector field $v = V_2 + a_4\, V_3 + a_5\, V_4$ and acting on v by $Ad(\exp(\varepsilon\, V_4))$ we obtain $\tilde{v} = V_2 + a_4\, V_3 + (a_5 + \frac{2\,a_4}{\beta}\,\varepsilon)\, V_4$. If $a_4 \neq 0$ then we can choose the group parameter $\varepsilon = -\frac{a_5\,\beta}{2\,a_4}$ and thus obtain $\hat{v} = V_2 + a_4\, V_3$. Moreover, if $a_4 = 0$ then we obtain $V_2 + a_5\, V_4$ with a_5 arbitrary. Thus, (ii) holds.

The rest of the one-dimensional subalgebras are spanned by vectors with $a_1 = a_2 = 0$ and $a_3 \neq 0$. Consider the vector field $v = V_3 + a_5\, V_4$ and acting on v by $Ad(\exp(\varepsilon\, V_4))$ we obtain $v''' = V_3 + (a_5 + \frac{2}{\beta}\,\varepsilon)\, V_4$. Choose the group parameter $\varepsilon = -\frac{a_5\,\beta}{2\,a_4}$ Then we obtain $v^{*} = V_3$. Similarly, we obtain that every one-dimensional subalgebra spanned by the vector fields v with $a_1 = a_2 = a_4 = 0$ and with $a_5 \neq 0$ is equivalent to a subalgebra spanned by V_4. Thus the proof of Theorem 4.5 is now complete. □

7.2 Absolutely and completely monotonic functions

In this subsection we provide a few definitions of absolutely and completely monotonic functions that we used in this thesis (see e.g. [117]).

Definition 8 *A function* $f : (a, b) \to \mathbb{R}$ *is said to be:*

(i) absolutely monotonic if $f^{(k)}(x) \geq 0$*, for* $x \in (a, b)$, $\quad k = 0, 1, 2, \ldots$

(ii) completely monotonic if $(-1)^k f^{(k)}(x) \geq 0$*, for* $x \in (a, b)$, $\quad k = 0, 1, 2, \ldots$

Remark 7.1 *From the definition above it follows that the sum and the product of any completely monotonic functions is also a completely monotonic function.*

Lemma 7.1 *If (i)* f_1 *is absolutely monotonic in the interval* (a, b)*, and (ii)* f_2 *is completely monotonic in the interval* (c, d) *with* $a < f_2((c, d)) < b$*, then* $f_1(f_2(x))$ *is completely monotonic in the interval* (c, d).

Ad	V_1	V_2	V_3	V_4	V_5	V_6	V_7	V_8
V_1	V_1	V_2	V_3	$V_4 - \varepsilon V_1$	V_5	$V_6 - \varepsilon V_5$	$V_7 - \varepsilon V_2$	$V_8 - \varepsilon V^*$
V_2	V_1	V_2	$V_3 - \varepsilon V_2$	V_4	$V_5 - \varepsilon V_1$	$V_6 - \varepsilon V^{**}$	V_7	$V_8 - \varepsilon V_7$
V_3	V_1	$e^{\varepsilon} V_2$	V_3	V_4	$e^{-\varepsilon} V_5$	$e^{-\varepsilon} V_6$	$e^{\varepsilon} V_7$	V_8
V_4	$e^{\varepsilon} V_1$	V_2	V_3	V_4	$e^{\varepsilon} V_5$	V_6	$e^{-\varepsilon} V_7$	$e^{-\varepsilon} V_8$
V_5	V_1	$V_2 + \varepsilon V_1$	$V_3 + \varepsilon V_5$	$V_4 - \varepsilon V_5$	V_5	V_6	$V_7 - \varepsilon(V_3 - V_4)$	$V_8 - \varepsilon V_6$
V_6	$V_1 + \varepsilon V_5$	$V_2 + \varepsilon V^{**}$	$V_3 + \varepsilon V_6$	V_4	V_5	V_6	$V_7 + \varepsilon V_8$	V_8
V_7	$V_1 + \varepsilon V_2$	V_2	$V_3 - \varepsilon V_7$	$V_4 + \varepsilon V_7$	$V_5 - \varepsilon(V_4 - V_3)$	$V_6 - \varepsilon V_8$	V_7	V_8
V_8	$V_1 + \varepsilon V^*$	$V_2 + \varepsilon V_7$	V_3	$V_4 + \varepsilon V_8$	$V_5 + \varepsilon V_6$	V_6	V_7	V_8

Table 7.1: Adjoint representation table for (4.34). The (i,j)-th entry is $Ad(\exp(\varepsilon V_i))\,V_j$, where $V^* = V_3 + 2\,V_4$ and $V^{**} = 2\,V_3 + V_4$

Ad	V_1	V_2	V_3	V_4	V_5	V_6	V_7	V_8
V_1	V_1	$e^{\varepsilon}\, V_2$	V_3	$e^{-\varepsilon}\, V_4$	V_5	$e^{-\varepsilon}\, V_6$	V_7	$e^{\varepsilon}\, V_8$
V_2	$V_1 - \varepsilon V_2$	V_2	V_3	$V_4 - \varepsilon V_3$	$V_5 + \frac{\varepsilon\alpha V_2}{\beta}$	$V_6 - \varepsilon V_5$	$V_7 - \varepsilon V_8$	V_8
V_3	V_1	V_2	V_3	V_4	$V_5 + \frac{\alpha\varepsilon V_3}{2\beta}$	$V_6 + \frac{\alpha\varepsilon V_4}{2\beta}$	$V_7 - V - \frac{4\varepsilon V_5}{\alpha}$	$V_8 + \frac{\varepsilon V_2}{\beta}$
V_4	$V_1 + \varepsilon V_4$	$V_2 + \varepsilon V_3$	V_3	V_4	$V_5 - \frac{\alpha\varepsilon V_4}{2\beta}$	V_6	$V_7 - \frac{2\varepsilon V_6}{\alpha}$	$V_8 + V + \frac{2\varepsilon V_5}{\alpha}$
V_5	V_1	$e^{-\frac{\alpha\varepsilon}{\beta}}\, V_2$	$e^{-\frac{\alpha\varepsilon}{2\beta}}\, V_3$	$e^{\frac{\alpha\varepsilon}{2\beta}}\, V_4$	V_5	$e^{\frac{\alpha\varepsilon}{\beta}}\, V_6$	$e^{\frac{\alpha\varepsilon}{2\beta}}\, V_7$	$e^{-\frac{\alpha\varepsilon}{2\beta}}\, V_8$
V_6	$V_1 + \varepsilon V_6$	$V_2 + \varepsilon V_5$	$V_3 - \frac{\alpha\varepsilon V_4}{2\beta}$	V_4	$V_5 - \frac{\alpha\varepsilon V_6}{\beta}$	V_6	V_7	$V_8 - \frac{\alpha\varepsilon V_7}{2\beta}$
V_7	V_1	$V_2 + \varepsilon V_8$	$V_3 + V + \frac{4\varepsilon V_5}{\alpha}$	$V_4 + \frac{2\varepsilon V_6}{\alpha}$	$V_5 - \frac{\alpha\varepsilon V_7}{2\beta}$	V_6	V_7	V_8
V_8	$V_1 - \varepsilon V_8$	V_2	$V_3 - \frac{\varepsilon V_2}{\beta}$	$V_4 - V - \frac{2\varepsilon V_5}{\alpha}$	$V_5 + \frac{\alpha\varepsilon V_8}{2\beta}$	$V_6 + \frac{\varepsilon\alpha V_7}{2\beta}$	V_7	V_8

Table 7.2: Adjoint representation table for (4.101). The (i,j)-th entry is $Ad(\exp(\varepsilon\, V_i))\, V_j$ where $V = \frac{3\varepsilon\, V_1}{\beta}$

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